



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:56 AM UTC

PDB ID : 3J6F / pdb_00003j6f
EMDB ID : EMD-5896
Title : Minimized average structure of GDP-bound dynamic microtubules
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 4.90 Å(reported)
Based on initial model : 1JFF

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

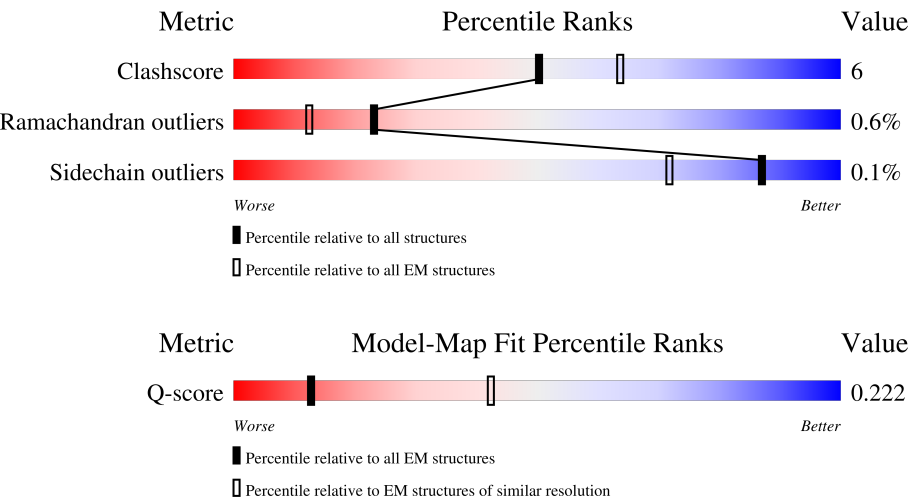
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1274 (4.40 - 5.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	34% 73%21%
1	C	439	42% 72%23%
1	E	439	40% 73%22%
1	G	439	49% 72%22%

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Mol	Chain	Length	Quality of chain
1	I	439	41% 73% 22% • •
1	K	439	49% 74% 21% • •
1	M	439	60% 73% 22% • •
1	O	439	54% 74% 21% • •
1	Q	439	63% 73% 21% • •
2	B	427	28% 76% 20% •
2	D	427	39% 76% 20% •
2	F	427	40% 76% 20% •
2	H	427	60% 76% 20% •
2	J	427	48% 76% 20% •
2	L	427	60% 76% 20% •
2	N	427	45% 75% 20% •
2	P	427	35% 74% 21% •
2	R	427	47% 74% 21% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60903 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	C	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	E	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	G	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	I	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	K	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	M	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	O	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	Q	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		

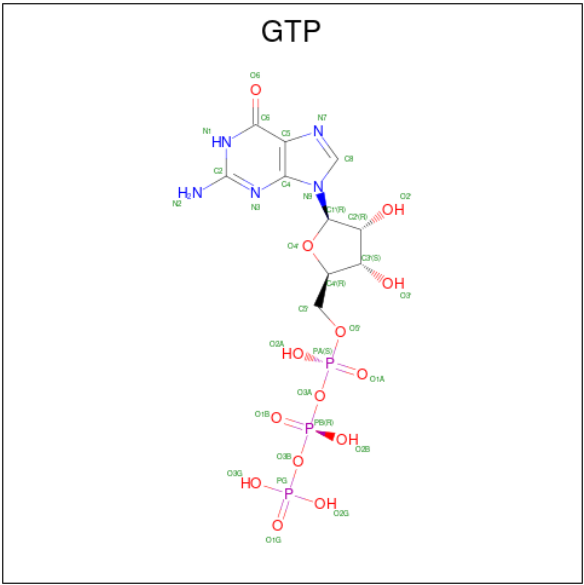
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550
C	265	GLY	ALA	conflict	UNP P02550
E	265	GLY	ALA	conflict	UNP P02550
G	265	GLY	ALA	conflict	UNP P02550
I	265	GLY	ALA	conflict	UNP P02550
K	265	GLY	ALA	conflict	UNP P02550
M	265	GLY	ALA	conflict	UNP P02550
O	265	GLY	ALA	conflict	UNP P02550
Q	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	D	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	F	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	H	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	J	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	L	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	N	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	P	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	R	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



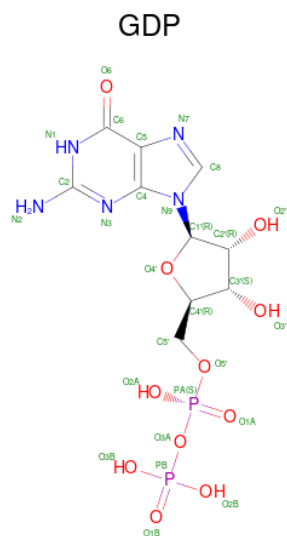
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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total 28	C 10	N 5	O 11	P 2	0
5	D	1	Total 28	C 10	N 5	O 11	P 2	0
5	F	1	Total 28	C 10	N 5	O 11	P 2	0
5	H	1	Total 28	C 10	N 5	O 11	P 2	0
5	J	1	Total 28	C 10	N 5	O 11	P 2	0
5	L	1	Total 28	C 10	N 5	O 11	P 2	0
5	N	1	Total 28	C 10	N 5	O 11	P 2	0
5	P	1	Total 28	C 10	N 5	O 11	P 2	0
5	R	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	4	Total O 4 4	0
6	C	4	Total O 4 4	0
6	E	4	Total O 4 4	0

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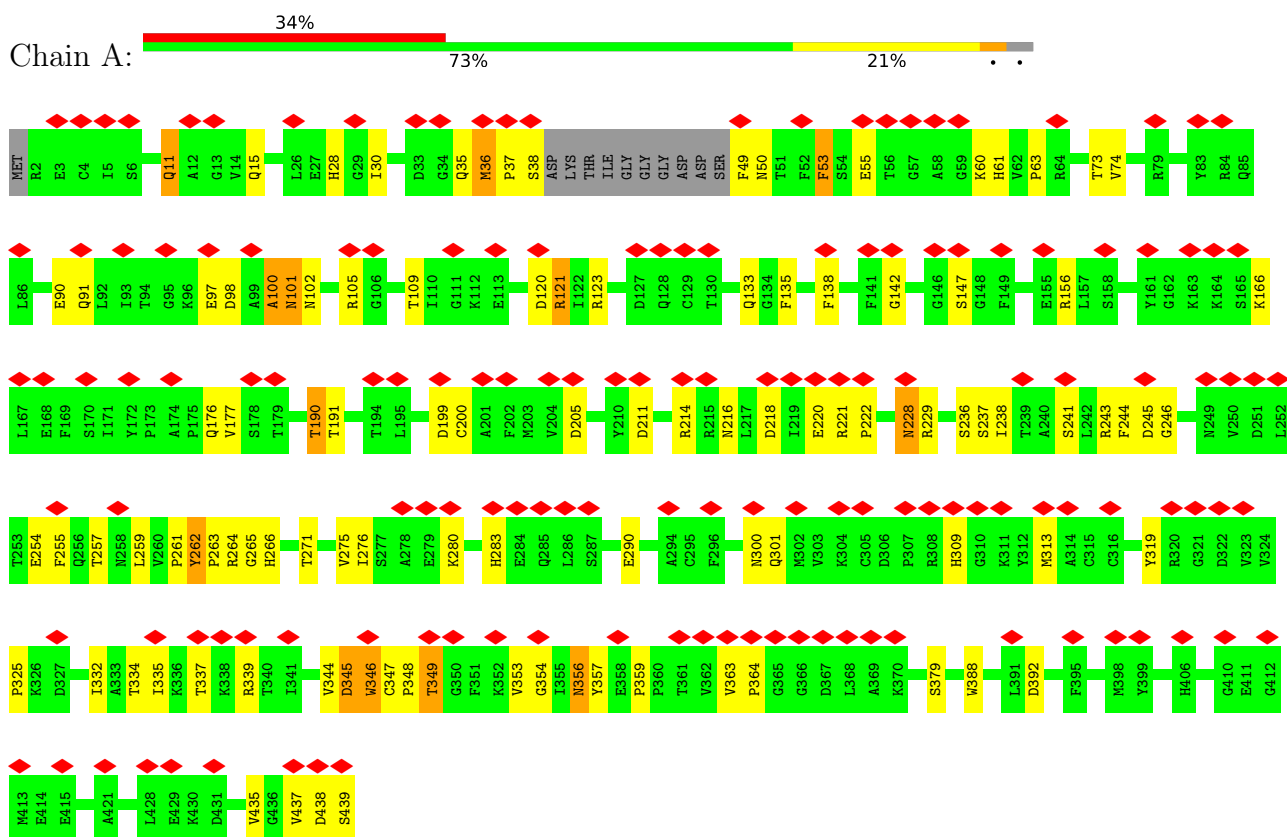
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Mol	Chain	Residues	Atoms		AltConf
6	G	4	Total 4	O 4	0
6	I	4	Total 4	O 4	0
6	K	4	Total 4	O 4	0
6	M	4	Total 4	O 4	0
6	O	4	Total 4	O 4	0
6	Q	4	Total 4	O 4	0

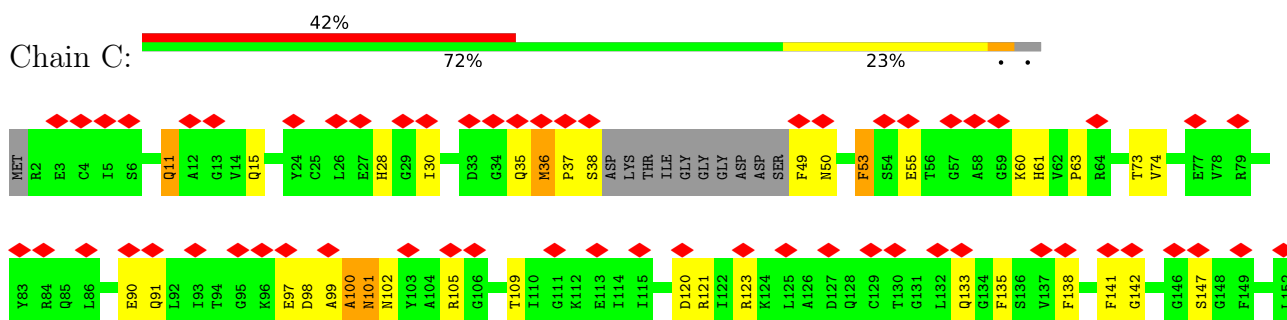
3 Residue-property plots

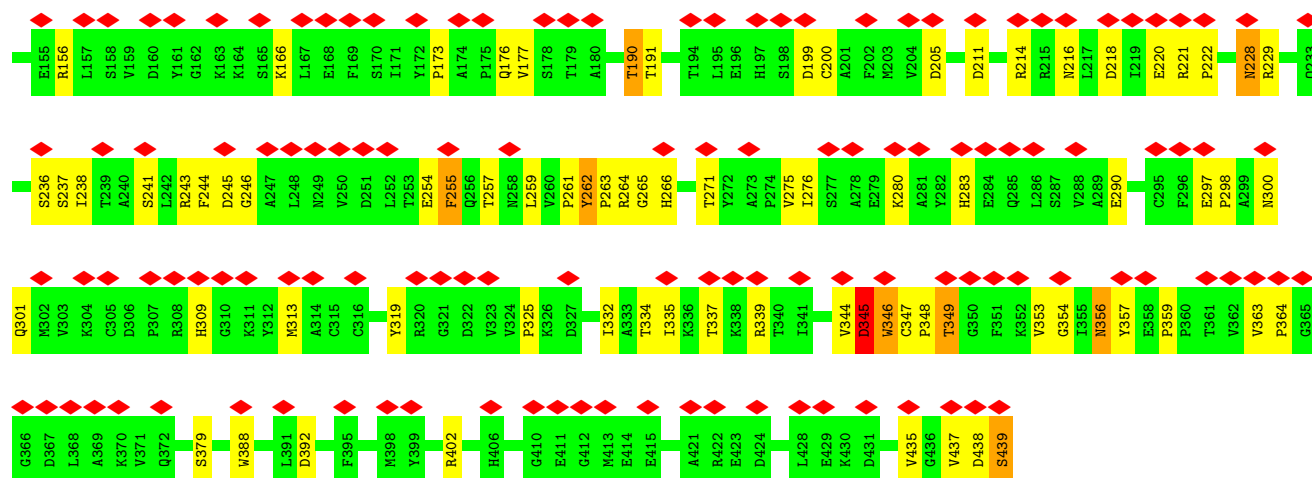
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tubulin alpha-1A chain

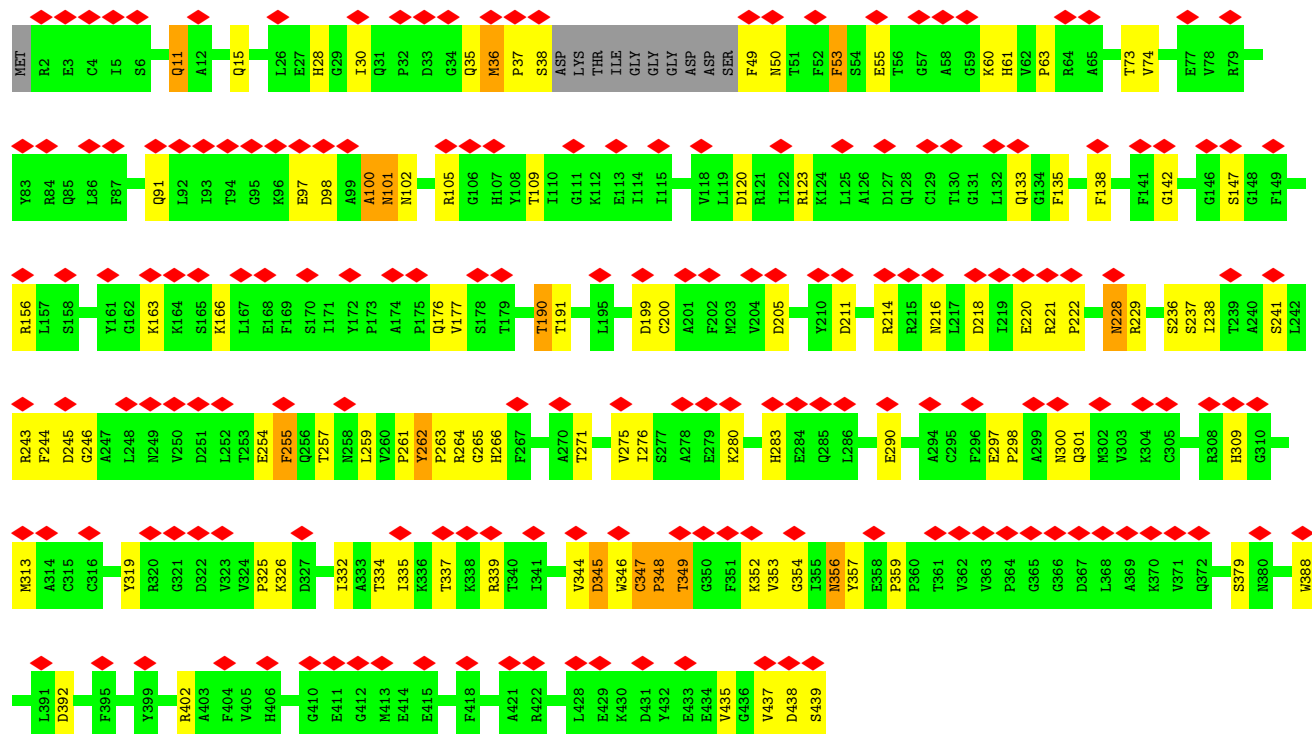
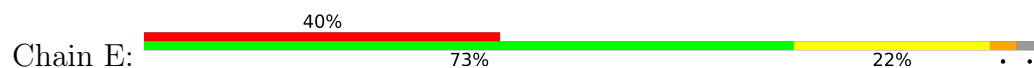


- Molecule 1: Tubulin alpha-1A chain

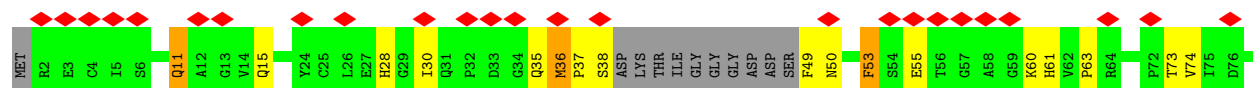


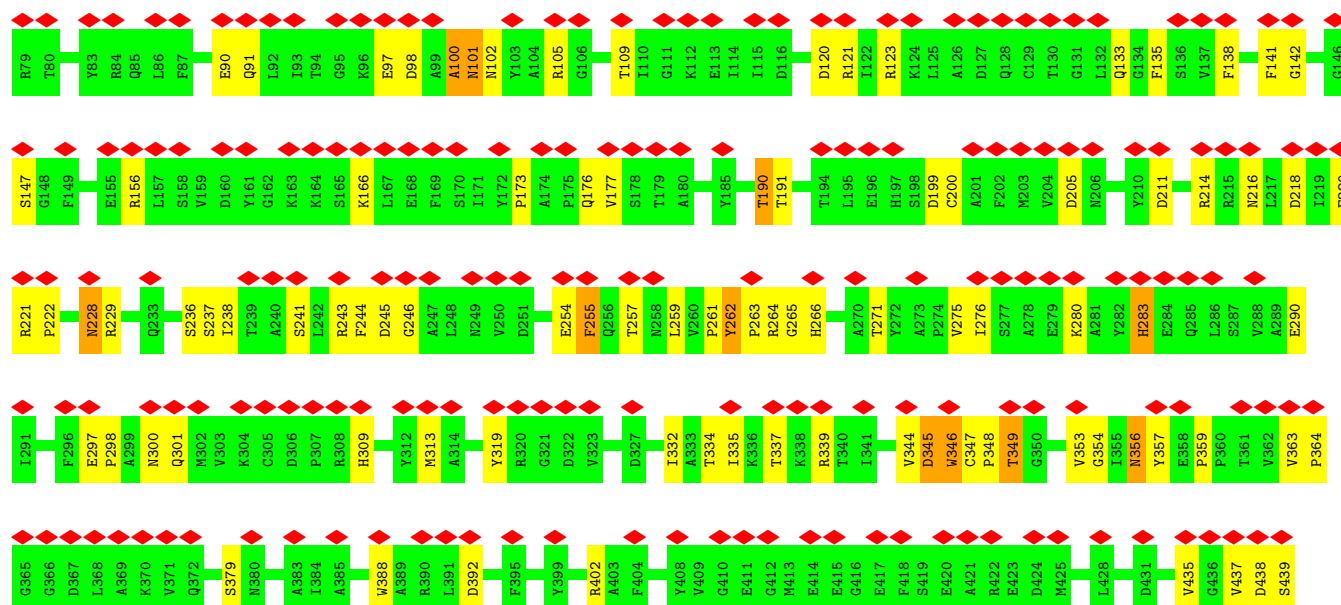


• Molecule 1: Tubulin alpha-1A chain

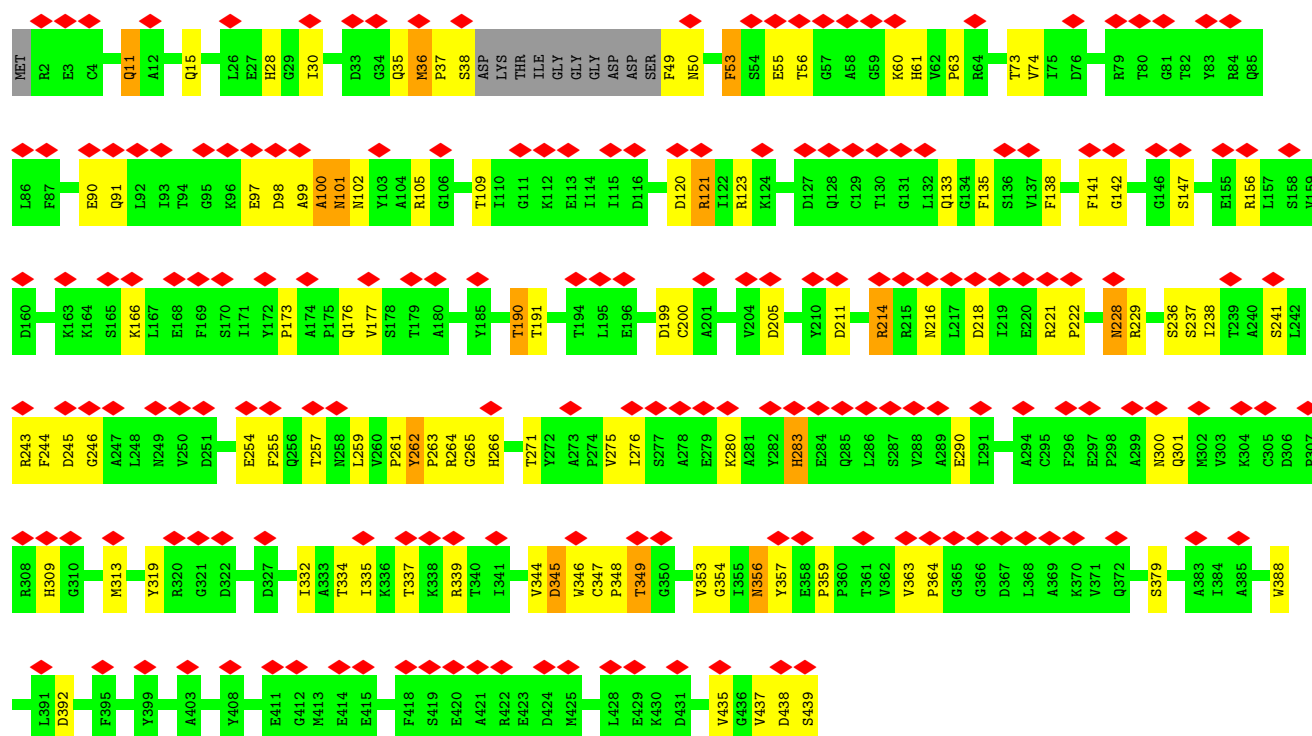
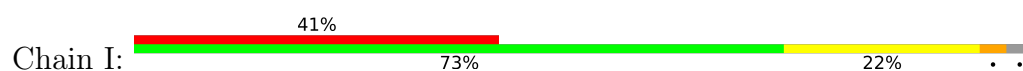


• Molecule 1: Tubulin alpha-1A chain

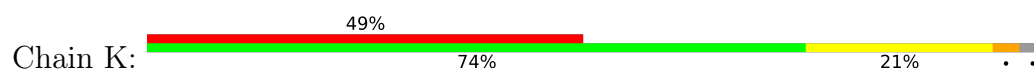


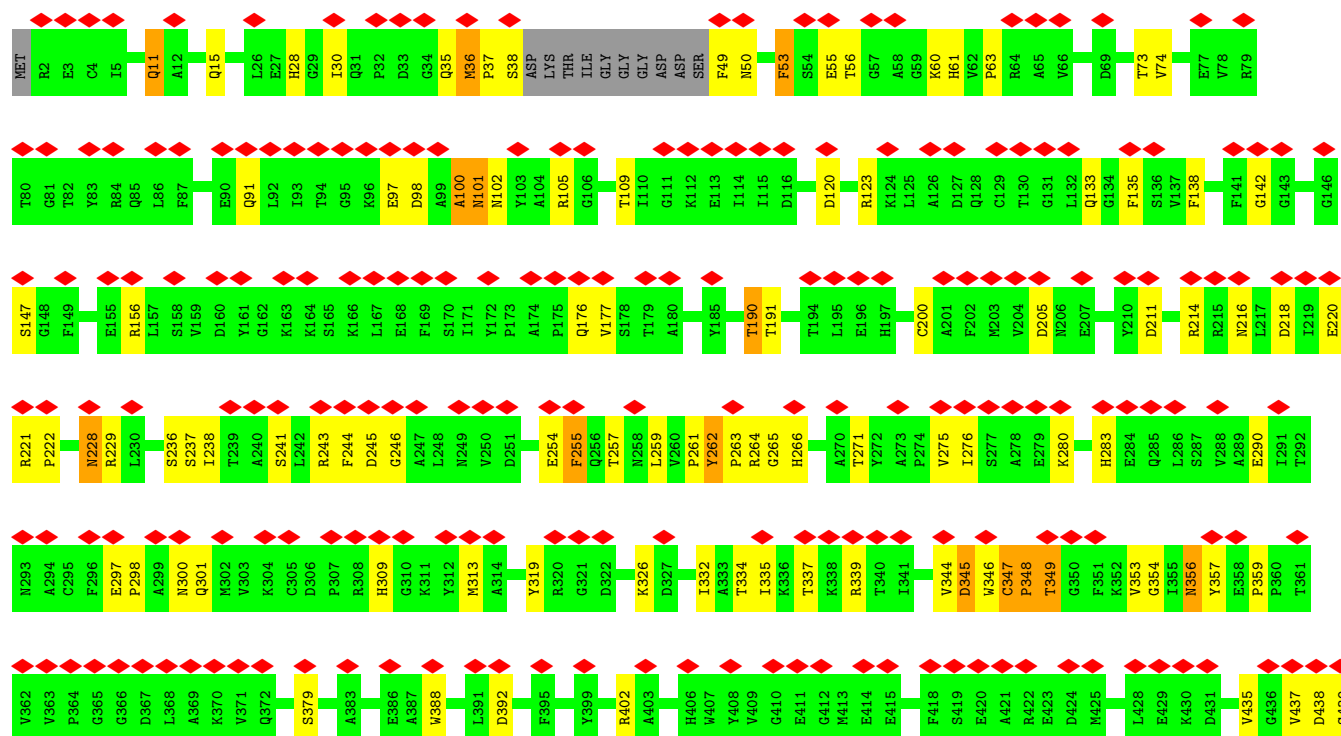


• Molecule 1: Tubulin alpha-1A chain

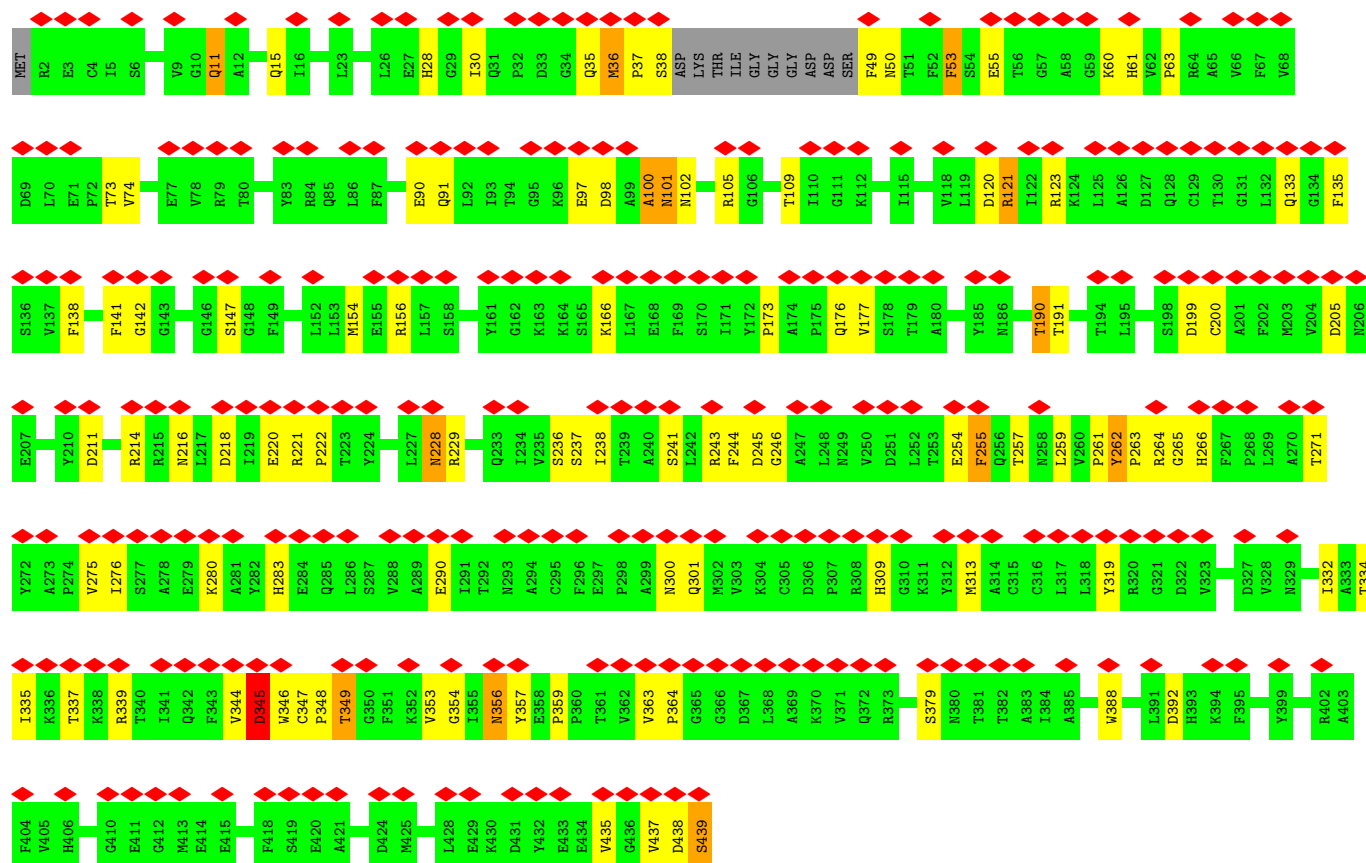
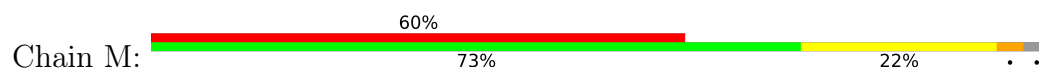


• Molecule 1: Tubulin alpha-1A chain





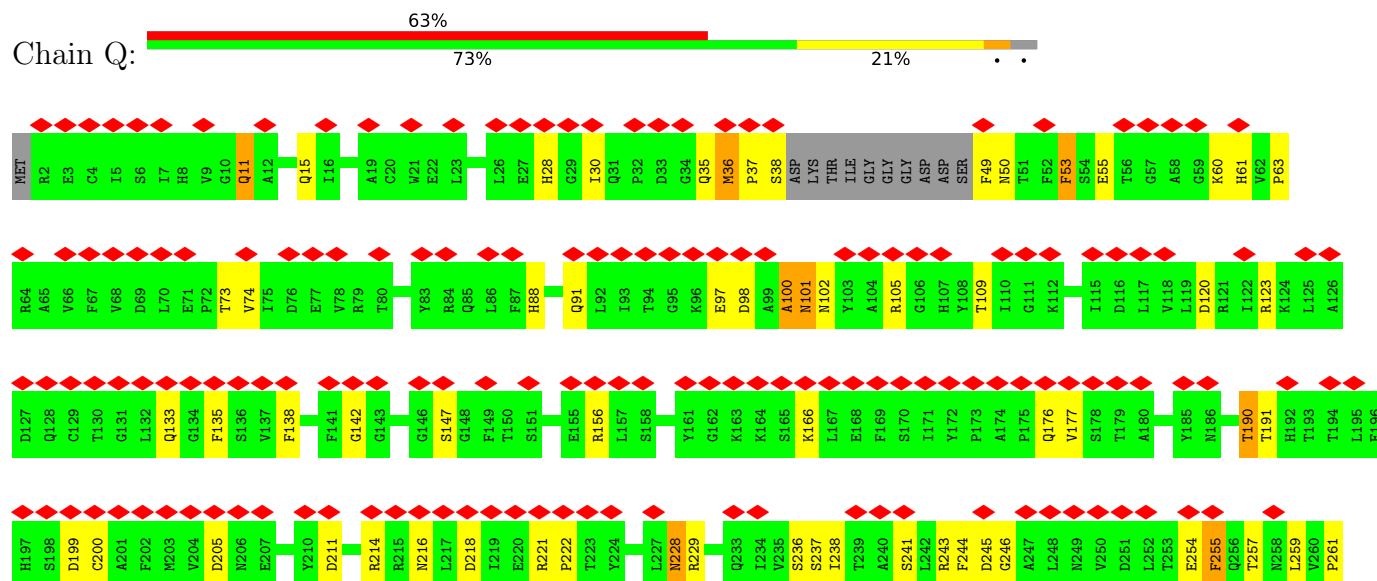
• Molecule 1: Tubulin alpha-1A chain

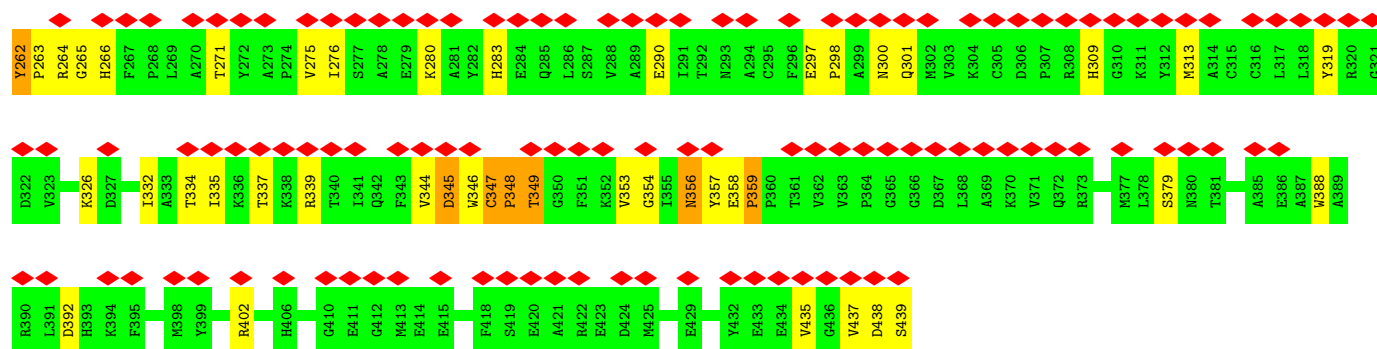


Chain O:

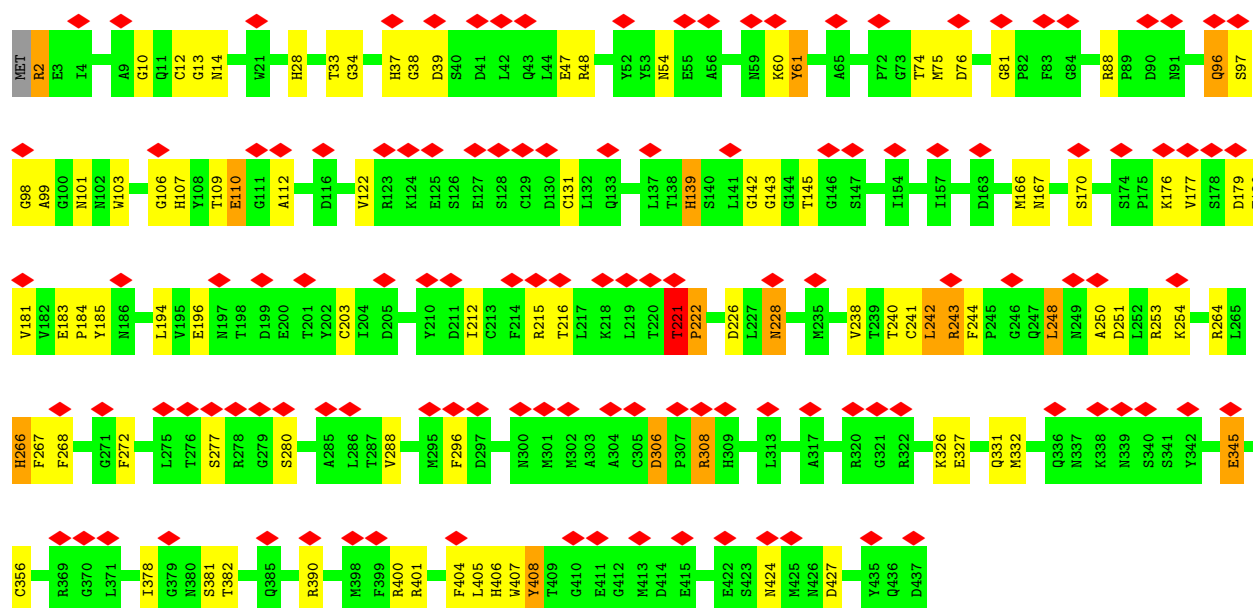
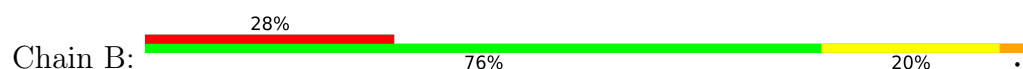


Chain Q:

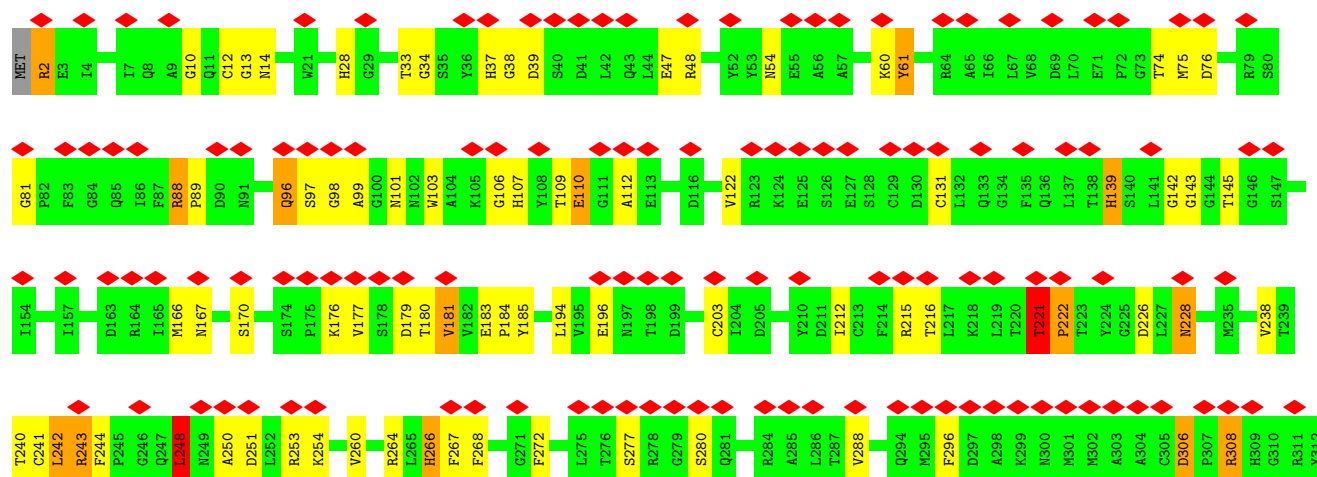
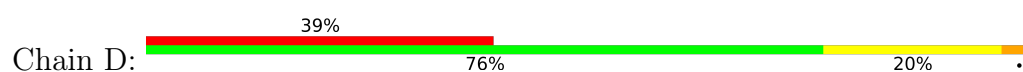


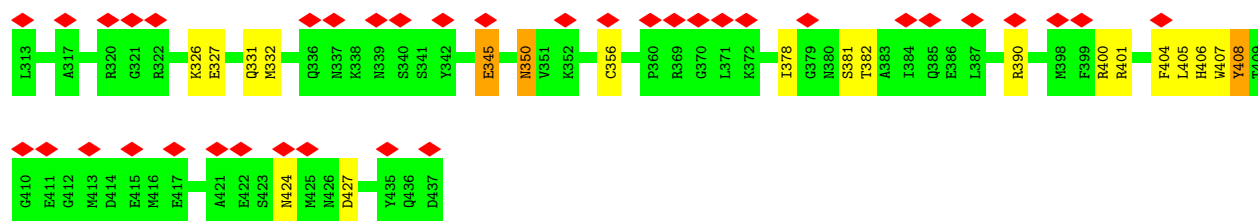


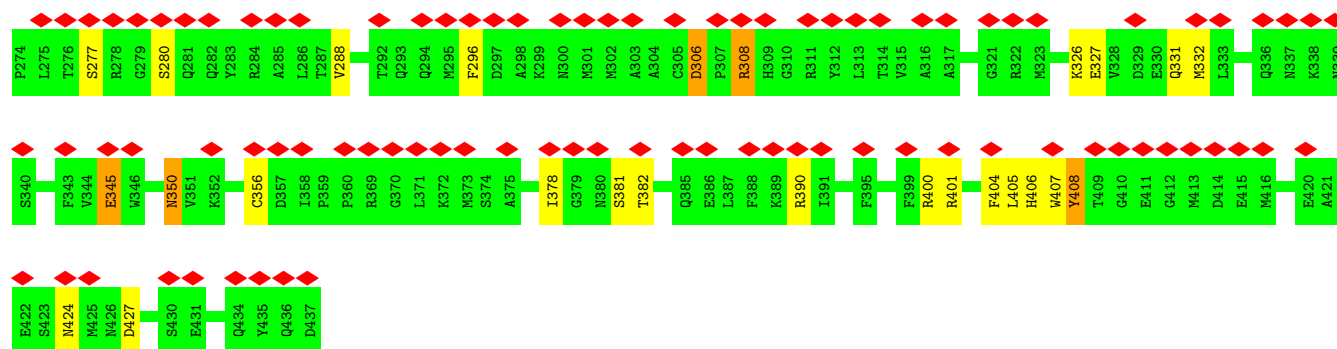
• Molecule 2: Tubulin beta chain



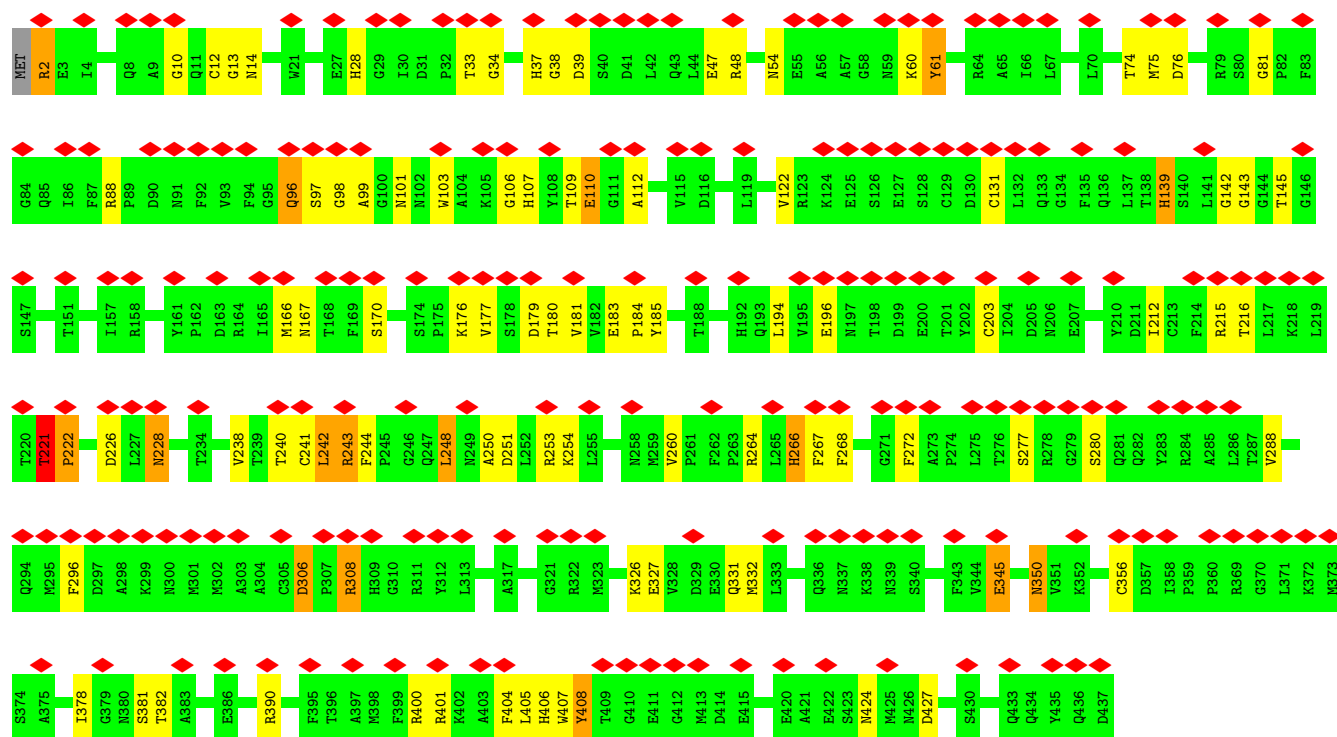
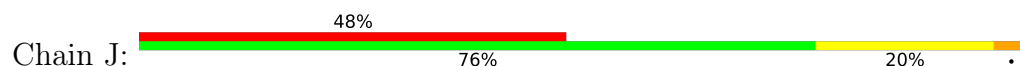
• Molecule 2: Tubulin beta chain



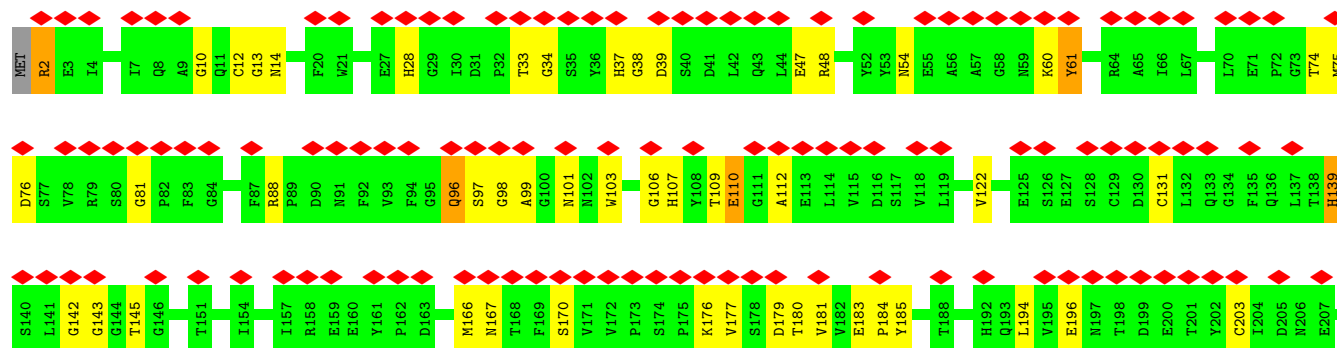
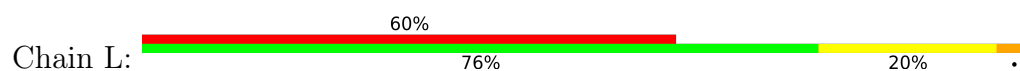


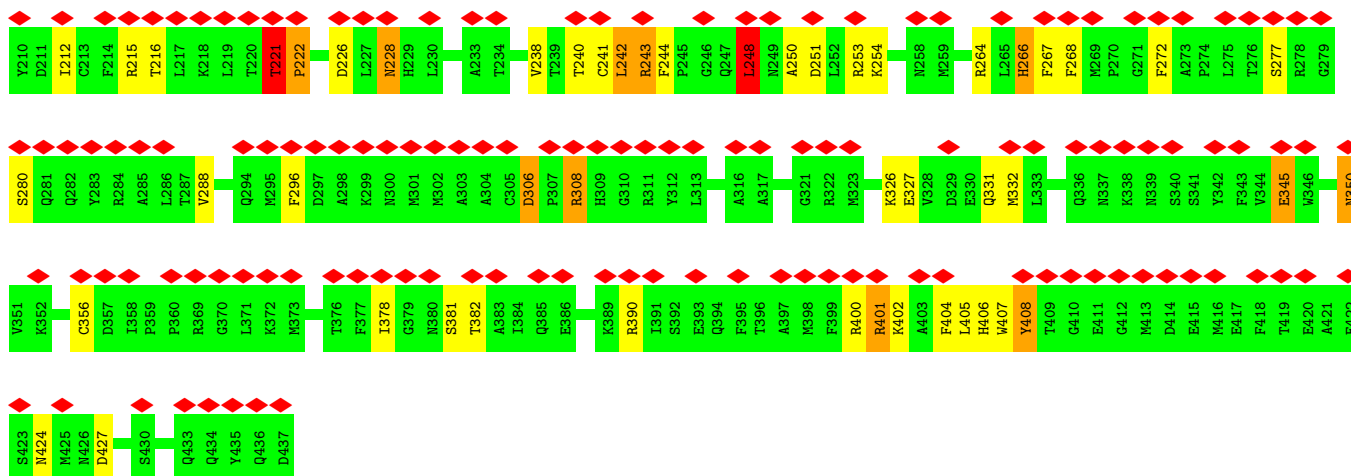


• Molecule 2: Tubulin beta chain

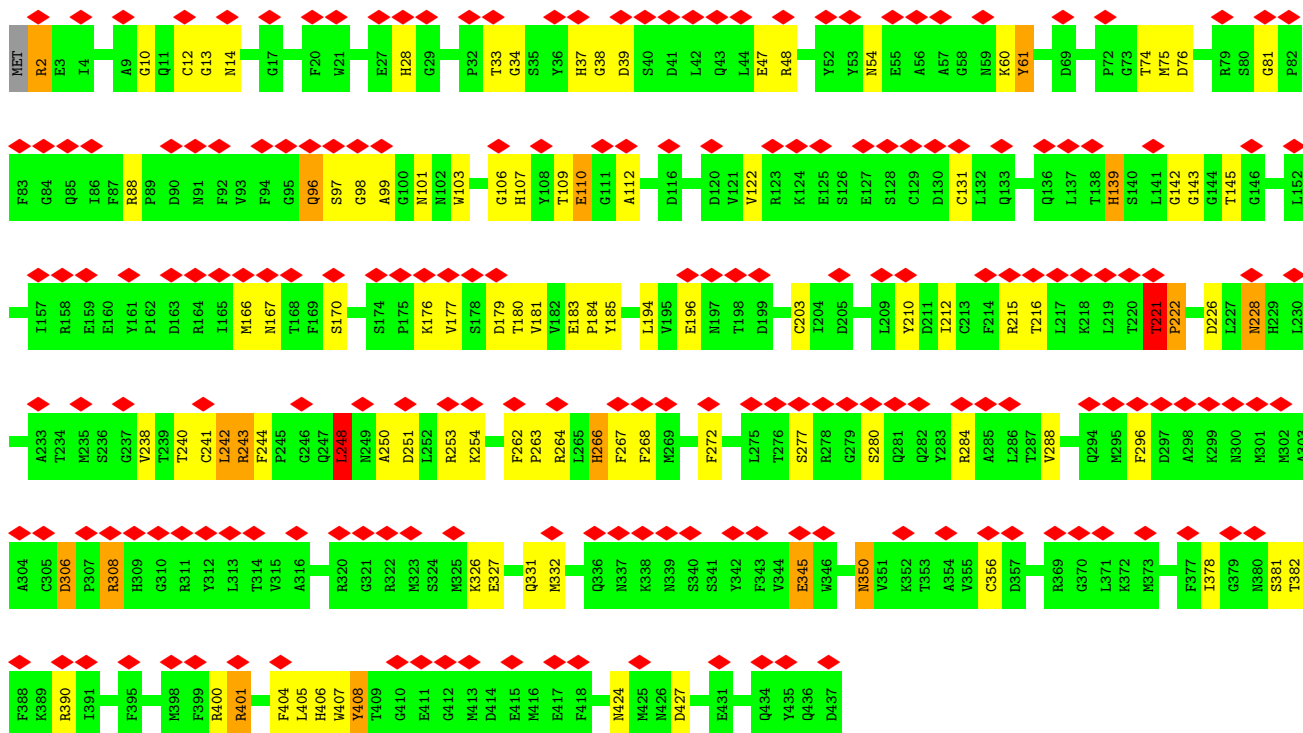
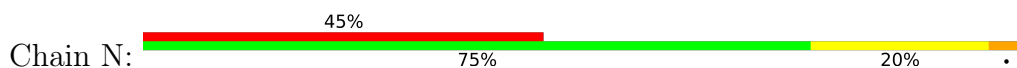


• Molecule 2: Tubulin beta chain

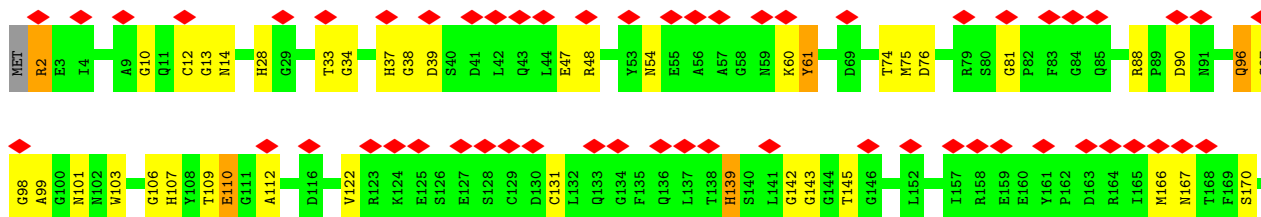
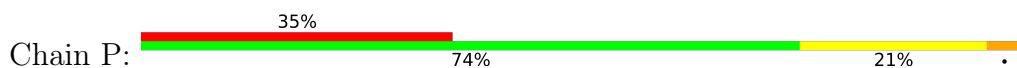


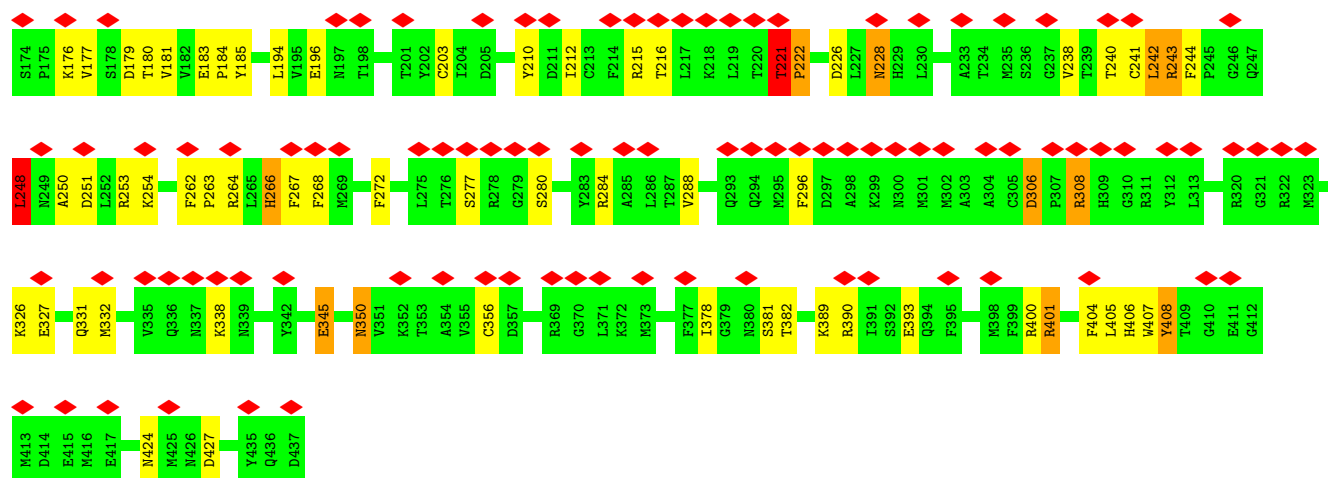


• Molecule 2: Tubulin beta chain

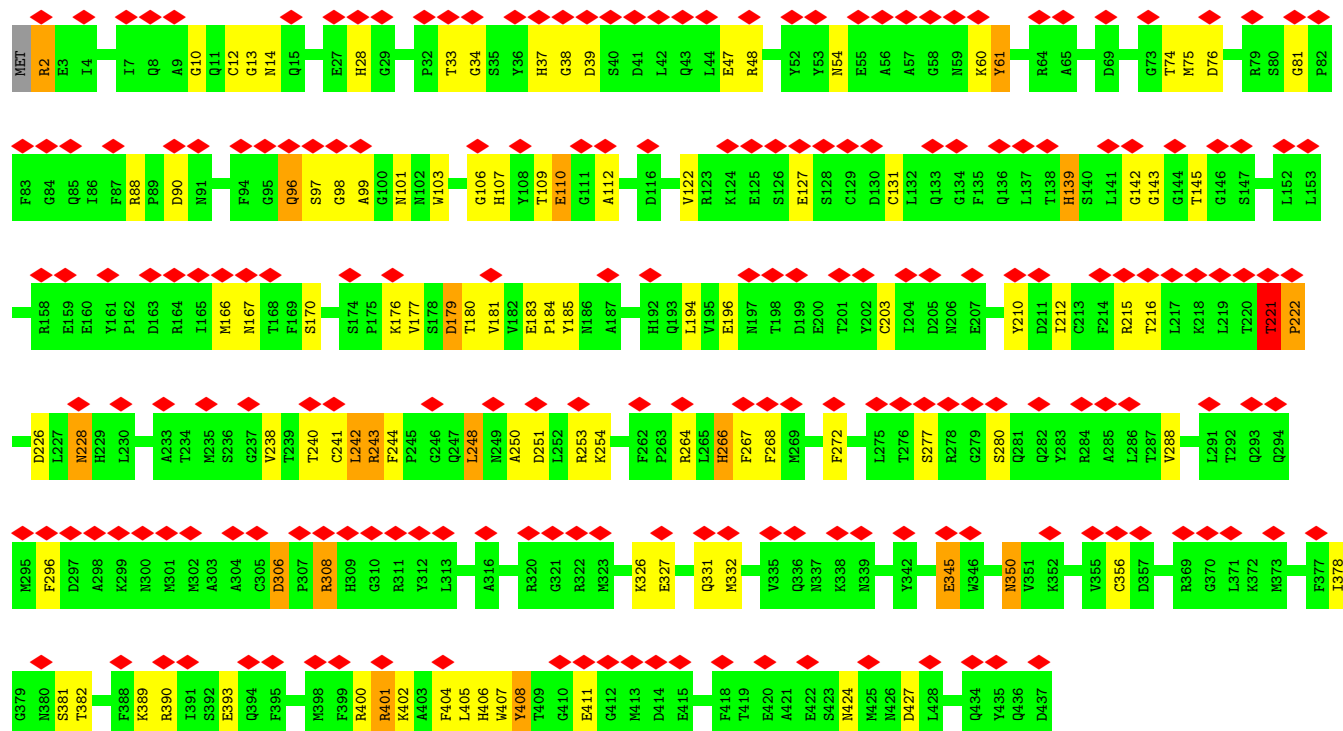
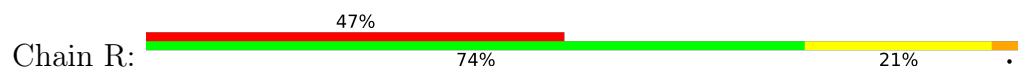


• Molecule 2: Tubulin beta chain





• Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	54445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	ctftilt	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	72000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.280	Depositor
Minimum map value	-4.672	Depositor
Average map value	0.528	Depositor
Map value standard deviation	1.926	Depositor
Recommended contour level	4	Depositor
Map size (Å)	191.4, 114.840004, 281.88	wwPDB
Map dimensions	110, 66, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7399999, 1.74, 1.74	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.48	31/3427 (0.9%)	1.80	80/4651 (1.7%)
1	C	1.48	32/3427 (0.9%)	1.80	79/4651 (1.7%)
1	E	1.48	31/3427 (0.9%)	1.80	79/4651 (1.7%)
1	G	1.48	32/3427 (0.9%)	1.80	79/4651 (1.7%)
1	I	1.48	31/3427 (0.9%)	1.80	81/4651 (1.7%)
1	K	1.48	31/3427 (0.9%)	1.80	79/4651 (1.7%)
1	M	1.48	32/3427 (0.9%)	1.80	80/4651 (1.7%)
1	O	1.48	32/3427 (0.9%)	1.81	79/4651 (1.7%)
1	Q	1.48	31/3427 (0.9%)	1.80	79/4651 (1.7%)
2	B	1.35	26/3427 (0.8%)	1.82	95/4642 (2.0%)
2	D	1.35	26/3427 (0.8%)	1.82	97/4642 (2.1%)
2	F	1.35	26/3427 (0.8%)	1.82	96/4642 (2.1%)
2	H	1.35	26/3427 (0.8%)	1.82	96/4642 (2.1%)
2	J	1.35	26/3427 (0.8%)	1.82	98/4642 (2.1%)
2	L	1.35	26/3427 (0.8%)	1.82	94/4642 (2.0%)
2	N	1.35	26/3427 (0.8%)	1.82	95/4642 (2.0%)
2	P	1.35	26/3427 (0.8%)	1.82	95/4642 (2.0%)
2	R	1.35	26/3427 (0.8%)	1.82	94/4642 (2.0%)
All	All	1.42	517/61686 (0.8%)	1.81	1575/83637 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
All	All	0	9

All (517) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	265	GLY	CA-C	-19.65	1.27	1.52
1	M	265	GLY	CA-C	-19.61	1.27	1.52
1	I	265	GLY	CA-C	-19.59	1.27	1.52
1	E	265	GLY	CA-C	-19.59	1.27	1.52
1	G	265	GLY	CA-C	-19.58	1.27	1.52
1	C	265	GLY	CA-C	-19.56	1.27	1.52
1	A	265	GLY	CA-C	-19.55	1.27	1.52
1	K	265	GLY	CA-C	-19.52	1.27	1.52
1	O	265	GLY	CA-C	-19.50	1.27	1.52
1	E	266	HIS	N-CA	-17.54	1.24	1.45
1	I	266	HIS	N-CA	-17.50	1.24	1.45
1	M	266	HIS	N-CA	-17.50	1.24	1.45
1	Q	266	HIS	N-CA	-17.49	1.24	1.45
1	A	266	HIS	N-CA	-17.48	1.24	1.45
1	C	266	HIS	N-CA	-17.46	1.24	1.45
1	O	266	HIS	N-CA	-17.46	1.24	1.45
1	G	266	HIS	N-CA	-17.44	1.24	1.45
1	K	266	HIS	N-CA	-17.44	1.24	1.45
2	J	250	ALA	N-CA	-15.95	1.20	1.46
2	N	250	ALA	N-CA	-15.94	1.20	1.46
2	H	250	ALA	N-CA	-15.93	1.20	1.46
2	D	250	ALA	N-CA	-15.93	1.20	1.46
2	B	250	ALA	N-CA	-15.92	1.20	1.46
2	F	250	ALA	N-CA	-15.91	1.20	1.46
2	L	250	ALA	N-CA	-15.91	1.20	1.46
2	R	250	ALA	N-CA	-15.91	1.20	1.46
2	P	250	ALA	N-CA	-15.90	1.20	1.46
1	I	264	ARG	CA-C	-14.18	1.33	1.53
1	E	264	ARG	CA-C	-14.17	1.33	1.53
1	A	264	ARG	CA-C	-14.16	1.33	1.53
1	G	264	ARG	CA-C	-14.16	1.33	1.53
1	O	264	ARG	CA-C	-14.15	1.33	1.53
1	M	264	ARG	CA-C	-14.15	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	264	ARG	CA-C	-14.14	1.33	1.53
1	Q	264	ARG	CA-C	-14.13	1.33	1.53
1	C	264	ARG	CA-C	-14.13	1.33	1.53
1	C	438	ASP	CA-C	-14.01	1.34	1.52
1	Q	438	ASP	CA-C	-14.00	1.34	1.52
1	E	438	ASP	CA-C	-13.98	1.34	1.52
1	O	438	ASP	CA-C	-13.98	1.34	1.52
1	K	438	ASP	CA-C	-13.97	1.34	1.52
1	G	438	ASP	CA-C	-13.96	1.34	1.52
1	A	438	ASP	CA-C	-13.95	1.34	1.52
1	I	438	ASP	CA-C	-13.95	1.34	1.52
1	M	438	ASP	CA-C	-13.94	1.34	1.52
2	H	96	GLN	CA-C	-13.32	1.35	1.52
2	D	96	GLN	CA-C	-13.31	1.35	1.52
2	P	96	GLN	CA-C	-13.31	1.35	1.52
2	B	96	GLN	CA-C	-13.28	1.35	1.52
2	L	96	GLN	CA-C	-13.27	1.35	1.52
2	J	96	GLN	CA-C	-13.25	1.35	1.52
2	R	96	GLN	CA-C	-13.22	1.35	1.52
2	F	96	GLN	CA-C	-12.71	1.35	1.52
2	N	96	GLN	CA-C	-12.69	1.35	1.52
1	G	348	PRO	N-CA	-11.96	1.33	1.46
1	I	348	PRO	N-CA	-11.96	1.33	1.46
1	C	348	PRO	N-CA	-11.96	1.33	1.46
1	K	348	PRO	N-CA	-11.93	1.33	1.46
1	M	348	PRO	N-CA	-11.90	1.33	1.46
1	A	348	PRO	N-CA	-11.90	1.33	1.46
1	E	348	PRO	N-CA	-11.89	1.33	1.46
1	Q	348	PRO	N-CA	-11.88	1.33	1.46
2	H	39	ASP	N-CA	-11.87	1.36	1.47
2	L	39	ASP	N-CA	-11.87	1.36	1.47
2	P	39	ASP	N-CA	-11.87	1.36	1.47
2	R	39	ASP	N-CA	-11.86	1.36	1.47
1	O	348	PRO	N-CA	-11.84	1.33	1.46
2	B	39	ASP	N-CA	-11.83	1.36	1.47
2	N	39	ASP	N-CA	-11.83	1.36	1.47
2	D	39	ASP	N-CA	-11.81	1.36	1.47
1	Q	348	PRO	CA-C	-11.76	1.38	1.52
2	J	39	ASP	N-CA	-11.75	1.36	1.47
1	K	348	PRO	CA-C	-11.74	1.38	1.52
1	I	348	PRO	CA-C	-11.73	1.38	1.52
1	C	348	PRO	CA-C	-11.72	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	39	ASP	N-CA	-11.71	1.36	1.47
1	G	348	PRO	CA-C	-11.71	1.38	1.52
1	A	348	PRO	CA-C	-11.70	1.38	1.52
1	O	348	PRO	CA-C	-11.69	1.38	1.52
1	M	348	PRO	CA-C	-11.65	1.38	1.52
1	E	348	PRO	CA-C	-11.65	1.38	1.52
1	Q	347	CYS	CA-C	-11.50	1.40	1.52
1	E	347	CYS	CA-C	-11.49	1.40	1.52
1	K	347	CYS	CA-C	-11.48	1.40	1.52
1	C	347	CYS	CA-C	-11.47	1.40	1.52
1	I	347	CYS	CA-C	-11.47	1.40	1.52
1	A	347	CYS	CA-C	-11.47	1.40	1.52
1	M	347	CYS	CA-C	-11.44	1.40	1.52
1	O	347	CYS	CA-C	-11.42	1.40	1.52
1	G	347	CYS	CA-C	-11.40	1.40	1.52
1	I	437	VAL	CA-C	-9.54	1.42	1.53
1	G	437	VAL	CA-C	-9.53	1.42	1.53
2	F	97	SER	N-CA	-9.51	1.34	1.46
2	R	97	SER	N-CA	-9.50	1.34	1.46
1	A	437	VAL	CA-C	-9.49	1.42	1.53
1	E	437	VAL	CA-C	-9.49	1.42	1.53
1	O	437	VAL	CA-C	-9.48	1.42	1.53
1	C	437	VAL	CA-C	-9.47	1.42	1.53
1	K	437	VAL	CA-C	-9.47	1.42	1.53
1	M	437	VAL	CA-C	-9.47	1.42	1.53
1	Q	437	VAL	CA-C	-9.46	1.42	1.53
2	P	97	SER	N-CA	-9.46	1.34	1.46
2	N	97	SER	N-CA	-9.45	1.35	1.46
2	H	97	SER	N-CA	-9.45	1.35	1.46
2	D	97	SER	N-CA	-9.45	1.35	1.46
2	B	97	SER	N-CA	-9.44	1.35	1.46
2	J	97	SER	N-CA	-9.43	1.35	1.46
2	L	97	SER	N-CA	-9.43	1.35	1.46
1	O	347	CYS	N-CA	-8.78	1.33	1.46
1	I	347	CYS	N-CA	-8.73	1.33	1.46
1	E	347	CYS	N-CA	-8.73	1.34	1.46
1	A	347	CYS	N-CA	-8.72	1.34	1.46
1	C	347	CYS	N-CA	-8.71	1.34	1.46
1	K	347	CYS	N-CA	-8.71	1.34	1.46
1	M	347	CYS	N-CA	-8.71	1.34	1.46
1	G	347	CYS	N-CA	-8.69	1.34	1.46
1	Q	347	CYS	N-CA	-8.69	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	242	LEU	N-CA	-8.65	1.34	1.46
2	H	242	LEU	N-CA	-8.63	1.35	1.46
2	P	242	LEU	N-CA	-8.63	1.35	1.46
2	L	242	LEU	N-CA	-8.63	1.35	1.46
2	B	242	LEU	N-CA	-8.62	1.35	1.46
2	F	242	LEU	N-CA	-8.62	1.35	1.46
2	R	242	LEU	N-CA	-8.61	1.35	1.46
2	D	242	LEU	N-CA	-8.57	1.35	1.46
2	J	242	LEU	N-CA	-8.55	1.35	1.46
1	G	345	ASP	CA-C	-8.16	1.41	1.52
1	E	345	ASP	CA-C	-8.12	1.41	1.52
1	O	345	ASP	CA-C	-8.09	1.42	1.52
1	A	345	ASP	CA-C	-8.08	1.42	1.52
1	K	345	ASP	CA-C	-8.08	1.42	1.52
1	Q	345	ASP	CA-C	-8.06	1.42	1.52
1	C	345	ASP	CA-C	-8.05	1.42	1.52
1	I	345	ASP	CA-C	-8.04	1.42	1.52
1	M	345	ASP	CA-C	-8.03	1.42	1.52
2	J	240	THR	CA-C	-8.02	1.41	1.52
2	B	240	THR	CA-C	-8.01	1.41	1.52
2	F	240	THR	CA-C	-8.01	1.41	1.52
2	P	240	THR	CA-C	-7.98	1.41	1.52
2	L	240	THR	CA-C	-7.98	1.41	1.52
2	R	240	THR	CA-C	-7.98	1.41	1.52
2	N	240	THR	CA-C	-7.98	1.41	1.52
2	D	240	THR	CA-C	-7.96	1.41	1.52
2	N	241	CYS	CA-C	-7.96	1.41	1.52
2	H	240	THR	CA-C	-7.95	1.41	1.52
2	P	241	CYS	CA-C	-7.95	1.41	1.52
1	I	100	ALA	CA-C	-7.94	1.43	1.53
2	D	241	CYS	CA-C	-7.93	1.41	1.52
2	H	241	CYS	CA-C	-7.93	1.41	1.52
2	J	241	CYS	CA-C	-7.92	1.41	1.52
1	C	100	ALA	CA-C	-7.91	1.43	1.53
2	B	241	CYS	CA-C	-7.91	1.41	1.52
1	Q	100	ALA	CA-C	-7.90	1.43	1.53
1	E	100	ALA	CA-C	-7.90	1.43	1.53
2	F	241	CYS	CA-C	-7.89	1.41	1.52
2	R	241	CYS	CA-C	-7.89	1.41	1.52
2	L	241	CYS	CA-C	-7.89	1.41	1.52
1	O	100	ALA	CA-C	-7.88	1.43	1.53
1	A	100	ALA	CA-C	-7.88	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	100	ALA	CA-C	-7.87	1.43	1.53
1	K	100	ALA	CA-C	-7.87	1.43	1.53
1	M	100	ALA	CA-C	-7.85	1.43	1.53
1	G	265	GLY	N-CA	-7.83	1.33	1.45
1	I	265	GLY	N-CA	-7.81	1.33	1.45
1	M	265	GLY	N-CA	-7.80	1.33	1.45
1	A	265	GLY	N-CA	-7.80	1.33	1.45
1	K	265	GLY	N-CA	-7.80	1.33	1.45
1	C	265	GLY	N-CA	-7.79	1.33	1.45
1	O	265	GLY	N-CA	-7.79	1.33	1.45
1	E	265	GLY	N-CA	-7.77	1.33	1.45
1	Q	265	GLY	N-CA	-7.77	1.33	1.45
1	C	344	VAL	CA-C	-7.75	1.43	1.52
1	Q	344	VAL	CA-C	-7.71	1.44	1.52
1	E	344	VAL	CA-C	-7.70	1.44	1.52
1	I	344	VAL	CA-C	-7.69	1.44	1.52
1	A	344	VAL	CA-C	-7.69	1.44	1.52
1	G	344	VAL	CA-C	-7.66	1.44	1.52
1	K	439	SER	N-CA	-7.66	1.31	1.46
1	E	439	SER	N-CA	-7.66	1.31	1.46
1	M	344	VAL	CA-C	-7.66	1.44	1.52
1	M	439	SER	N-CA	-7.65	1.31	1.46
1	I	439	SER	N-CA	-7.64	1.31	1.46
1	G	439	SER	N-CA	-7.63	1.31	1.46
1	C	439	SER	N-CA	-7.63	1.31	1.46
1	A	439	SER	N-CA	-7.62	1.31	1.46
1	Q	439	SER	N-CA	-7.62	1.31	1.46
1	K	344	VAL	CA-C	-7.62	1.44	1.52
1	O	439	SER	N-CA	-7.61	1.31	1.46
1	O	344	VAL	CA-C	-7.60	1.44	1.52
2	F	38	GLY	CA-C	-7.59	1.41	1.51
2	H	38	GLY	CA-C	-7.58	1.41	1.51
2	J	38	GLY	CA-C	-7.55	1.41	1.51
2	D	38	GLY	CA-C	-7.55	1.41	1.51
2	R	38	GLY	CA-C	-7.54	1.41	1.51
2	B	38	GLY	CA-C	-7.54	1.41	1.51
2	L	38	GLY	CA-C	-7.54	1.41	1.51
2	P	38	GLY	CA-C	-7.52	1.41	1.51
2	N	38	GLY	CA-C	-7.51	1.41	1.51
1	C	346	TRP	N-CA	-7.09	1.36	1.46
1	O	346	TRP	N-CA	-7.09	1.36	1.46
1	K	346	TRP	N-CA	-7.09	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	346	TRP	N-CA	-7.09	1.37	1.46
2	L	97	SER	CA-C	-7.09	1.45	1.53
1	G	346	TRP	N-CA	-7.08	1.37	1.46
1	M	346	TRP	N-CA	-7.07	1.37	1.46
1	I	346	TRP	N-CA	-7.07	1.37	1.46
2	D	97	SER	CA-C	-7.06	1.45	1.53
1	A	346	TRP	N-CA	-7.06	1.37	1.46
1	Q	346	TRP	N-CA	-7.04	1.37	1.46
2	H	97	SER	CA-C	-7.03	1.45	1.53
2	B	97	SER	CA-C	-7.01	1.45	1.53
2	R	97	SER	CA-C	-7.00	1.45	1.53
2	F	97	SER	CA-C	-7.00	1.45	1.53
2	J	97	SER	CA-C	-7.00	1.45	1.53
2	P	97	SER	CA-C	-6.99	1.45	1.53
2	N	97	SER	CA-C	-6.98	1.45	1.53
1	I	438	ASP	N-CA	-6.88	1.37	1.45
1	Q	438	ASP	N-CA	-6.88	1.37	1.45
1	O	438	ASP	N-CA	-6.87	1.37	1.45
1	E	438	ASP	N-CA	-6.84	1.37	1.45
1	A	438	ASP	N-CA	-6.83	1.37	1.45
1	K	438	ASP	N-CA	-6.83	1.37	1.45
1	C	438	ASP	N-CA	-6.82	1.37	1.45
1	M	438	ASP	N-CA	-6.80	1.37	1.45
1	G	438	ASP	N-CA	-6.80	1.37	1.45
2	P	222	PRO	N-CA	-6.67	1.38	1.47
2	H	222	PRO	N-CA	-6.67	1.38	1.47
2	J	222	PRO	N-CA	-6.63	1.38	1.47
2	L	222	PRO	N-CA	-6.62	1.38	1.47
2	B	222	PRO	N-CA	-6.61	1.38	1.47
2	D	222	PRO	N-CA	-6.61	1.38	1.47
2	N	222	PRO	N-CA	-6.59	1.38	1.47
1	K	97	GLU	CA-C	-6.59	1.44	1.52
2	D	250	ALA	CA-C	-6.59	1.46	1.53
1	O	97	GLU	CA-C	-6.58	1.44	1.52
2	L	250	ALA	CA-C	-6.58	1.46	1.53
2	R	222	PRO	N-CA	-6.57	1.39	1.47
1	Q	97	GLU	CA-C	-6.57	1.44	1.52
2	L	243	ARG	N-CA	-6.56	1.38	1.46
2	F	222	PRO	N-CA	-6.56	1.39	1.47
2	R	243	ARG	N-CA	-6.56	1.38	1.46
2	H	250	ALA	CA-C	-6.55	1.46	1.53
2	F	250	ALA	CA-C	-6.55	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	250	ALA	CA-C	-6.55	1.46	1.53
2	P	250	ALA	CA-C	-6.54	1.46	1.53
1	A	97	GLU	CA-C	-6.54	1.44	1.52
2	R	250	ALA	CA-C	-6.53	1.46	1.53
2	B	243	ARG	N-CA	-6.52	1.38	1.46
1	E	97	GLU	CA-C	-6.52	1.44	1.52
2	N	243	ARG	N-CA	-6.51	1.38	1.46
2	F	243	ARG	N-CA	-6.51	1.38	1.46
2	D	243	ARG	N-CA	-6.49	1.38	1.46
1	I	97	GLU	CA-C	-6.49	1.44	1.52
1	M	97	GLU	CA-C	-6.49	1.44	1.52
2	N	250	ALA	CA-C	-6.49	1.46	1.53
1	G	97	GLU	CA-C	-6.48	1.44	1.52
2	P	243	ARG	N-CA	-6.48	1.38	1.46
1	C	97	GLU	CA-C	-6.47	1.44	1.52
1	M	37	PRO	CA-C	-6.47	1.45	1.52
2	H	243	ARG	N-CA	-6.47	1.38	1.46
2	J	250	ALA	CA-C	-6.46	1.46	1.53
1	G	37	PRO	CA-C	-6.45	1.45	1.52
1	C	37	PRO	CA-C	-6.44	1.45	1.52
2	J	243	ARG	N-CA	-6.44	1.38	1.46
1	I	37	PRO	CA-C	-6.43	1.45	1.52
1	A	37	PRO	CA-C	-6.42	1.45	1.52
1	E	37	PRO	CA-C	-6.41	1.45	1.52
1	O	37	PRO	CA-C	-6.41	1.45	1.52
1	K	37	PRO	CA-C	-6.41	1.45	1.52
1	Q	37	PRO	CA-C	-6.38	1.45	1.52
2	L	107	HIS	CA-C	-6.38	1.45	1.52
2	J	107	HIS	CA-C	-6.36	1.45	1.52
2	D	107	HIS	CA-C	-6.34	1.45	1.52
2	N	107	HIS	CA-C	-6.33	1.45	1.52
2	B	107	HIS	CA-C	-6.33	1.45	1.52
2	P	107	HIS	CA-C	-6.33	1.45	1.52
2	R	107	HIS	CA-C	-6.31	1.45	1.52
2	F	107	HIS	CA-C	-6.31	1.45	1.52
2	H	107	HIS	CA-C	-6.31	1.45	1.52
1	C	265	GLY	C-N	-6.04	1.24	1.33
1	G	265	GLY	C-N	-6.04	1.24	1.33
1	O	265	GLY	C-N	-6.03	1.24	1.33
1	M	265	GLY	C-N	-6.02	1.24	1.33
1	A	265	GLY	C-N	-6.02	1.24	1.33
1	I	265	GLY	C-N	-6.01	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	265	GLY	C-N	-6.01	1.24	1.33
1	E	265	GLY	C-N	-6.00	1.24	1.33
2	H	241	CYS	N-CA	-6.00	1.38	1.46
2	D	241	CYS	N-CA	-5.99	1.38	1.46
1	Q	265	GLY	C-N	-5.99	1.24	1.33
1	E	262	TYR	N-CA	-5.97	1.41	1.46
2	N	241	CYS	N-CA	-5.97	1.38	1.46
2	R	241	CYS	N-CA	-5.97	1.38	1.46
2	B	241	CYS	N-CA	-5.97	1.38	1.46
1	I	262	TYR	N-CA	-5.97	1.41	1.46
2	F	241	CYS	N-CA	-5.96	1.38	1.46
1	Q	346	TRP	CA-C	-5.96	1.44	1.52
2	D	177	VAL	CA-C	-5.95	1.47	1.52
2	L	241	CYS	N-CA	-5.95	1.38	1.46
1	E	346	TRP	CA-C	-5.94	1.44	1.52
2	J	241	CYS	N-CA	-5.93	1.38	1.46
1	M	262	TYR	N-CA	-5.93	1.41	1.46
2	H	177	VAL	CA-C	-5.93	1.47	1.52
1	G	262	TYR	N-CA	-5.91	1.41	1.46
1	O	262	TYR	N-CA	-5.91	1.41	1.46
2	R	177	VAL	CA-C	-5.91	1.47	1.52
1	C	262	TYR	N-CA	-5.91	1.41	1.46
2	P	241	CYS	N-CA	-5.91	1.38	1.46
1	A	262	TYR	N-CA	-5.90	1.41	1.46
1	K	346	TRP	CA-C	-5.90	1.44	1.52
2	F	177	VAL	CA-C	-5.89	1.47	1.52
1	A	346	TRP	CA-C	-5.89	1.44	1.52
1	M	346	TRP	CA-C	-5.88	1.44	1.52
1	G	346	TRP	CA-C	-5.88	1.44	1.52
1	I	346	TRP	CA-C	-5.88	1.44	1.52
1	K	262	TYR	N-CA	-5.88	1.41	1.46
2	B	177	VAL	CA-C	-5.87	1.47	1.52
2	P	177	VAL	CA-C	-5.86	1.47	1.52
1	O	346	TRP	CA-C	-5.86	1.44	1.52
1	C	346	TRP	CA-C	-5.86	1.44	1.52
2	H	405	LEU	CA-C	-5.85	1.44	1.52
2	J	177	VAL	CA-C	-5.85	1.47	1.52
2	R	405	LEU	CA-C	-5.85	1.44	1.52
2	N	177	VAL	CA-C	-5.84	1.47	1.52
2	L	177	VAL	CA-C	-5.83	1.47	1.52
2	L	405	LEU	CA-C	-5.83	1.44	1.52
2	B	405	LEU	CA-C	-5.82	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	405	LEU	CA-C	-5.81	1.44	1.52
2	P	405	LEU	CA-C	-5.81	1.44	1.52
2	L	180	THR	CA-C	-5.80	1.45	1.52
2	D	405	LEU	CA-C	-5.80	1.44	1.52
2	F	405	LEU	CA-C	-5.79	1.44	1.52
2	H	180	THR	CA-C	-5.79	1.45	1.52
2	N	405	LEU	CA-C	-5.79	1.44	1.52
1	Q	262	TYR	N-CA	-5.79	1.42	1.46
2	R	180	THR	CA-C	-5.78	1.45	1.52
2	P	180	THR	CA-C	-5.77	1.45	1.52
2	J	180	THR	CA-C	-5.77	1.45	1.52
2	B	180	THR	CA-C	-5.75	1.45	1.52
2	N	180	THR	CA-C	-5.75	1.45	1.52
2	L	248	LEU	CA-C	-5.74	1.44	1.53
2	D	180	THR	CA-C	-5.73	1.45	1.52
2	J	110	GLU	CA-C	-5.73	1.45	1.52
1	E	38	SER	CA-C	-5.73	1.41	1.52
2	N	248	LEU	CA-C	-5.73	1.44	1.53
2	F	248	LEU	CA-C	-5.72	1.44	1.53
2	F	180	THR	CA-C	-5.72	1.45	1.52
2	P	248	LEU	CA-C	-5.72	1.44	1.53
1	O	38	SER	CA-C	-5.72	1.41	1.52
2	R	110	GLU	CA-C	-5.71	1.45	1.52
1	G	38	SER	CA-C	-5.71	1.41	1.52
2	H	110	GLU	CA-C	-5.71	1.45	1.52
2	D	248	LEU	CA-C	-5.71	1.44	1.53
2	D	110	GLU	CA-C	-5.70	1.45	1.52
1	I	38	SER	CA-C	-5.70	1.41	1.52
2	P	110	GLU	CA-C	-5.70	1.45	1.52
1	A	38	SER	CA-C	-5.70	1.41	1.52
2	J	248	LEU	CA-C	-5.70	1.44	1.53
1	M	37	PRO	N-CA	-5.70	1.41	1.47
2	B	248	LEU	CA-C	-5.70	1.44	1.53
2	H	248	LEU	CA-C	-5.70	1.44	1.53
1	Q	38	SER	CA-C	-5.70	1.41	1.52
2	B	110	GLU	CA-C	-5.69	1.45	1.52
2	R	248	LEU	CA-C	-5.69	1.44	1.53
2	D	242	LEU	CA-C	-5.69	1.45	1.52
1	M	38	SER	CA-C	-5.69	1.41	1.52
2	F	110	GLU	CA-C	-5.68	1.45	1.52
1	K	38	SER	CA-C	-5.68	1.41	1.52
1	C	38	SER	CA-C	-5.67	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	110	GLU	CA-C	-5.67	1.45	1.52
2	L	110	GLU	CA-C	-5.67	1.45	1.52
2	J	242	LEU	CA-C	-5.65	1.45	1.52
2	H	242	LEU	CA-C	-5.65	1.45	1.52
2	F	242	LEU	CA-C	-5.64	1.45	1.52
1	G	349	THR	N-CA	-5.63	1.39	1.46
2	N	242	LEU	CA-C	-5.63	1.45	1.52
2	B	242	LEU	CA-C	-5.63	1.45	1.52
1	C	37	PRO	N-CA	-5.63	1.41	1.47
1	O	37	PRO	N-CA	-5.63	1.41	1.47
1	K	37	PRO	N-CA	-5.63	1.41	1.47
2	L	242	LEU	CA-C	-5.63	1.45	1.52
1	Q	349	THR	N-CA	-5.62	1.39	1.46
1	C	264	ARG	C-N	-5.62	1.24	1.33
1	A	37	PRO	N-CA	-5.62	1.41	1.47
1	I	37	PRO	N-CA	-5.62	1.41	1.47
1	C	349	THR	N-CA	-5.61	1.39	1.46
1	I	264	ARG	C-N	-5.61	1.24	1.33
1	G	37	PRO	N-CA	-5.61	1.41	1.47
2	P	242	LEU	CA-C	-5.60	1.45	1.52
1	E	349	THR	N-CA	-5.60	1.39	1.46
1	E	37	PRO	N-CA	-5.59	1.41	1.47
1	Q	264	ARG	C-N	-5.59	1.24	1.33
1	G	264	ARG	C-N	-5.59	1.24	1.33
2	R	242	LEU	CA-C	-5.59	1.45	1.52
1	K	264	ARG	C-N	-5.58	1.24	1.33
1	A	349	THR	N-CA	-5.58	1.39	1.46
1	I	349	THR	N-CA	-5.57	1.39	1.46
1	O	264	ARG	C-N	-5.57	1.24	1.33
1	K	349	THR	N-CA	-5.57	1.39	1.46
1	E	264	ARG	C-N	-5.56	1.24	1.33
1	A	264	ARG	C-N	-5.56	1.24	1.33
1	Q	37	PRO	N-CA	-5.56	1.41	1.47
1	M	349	THR	N-CA	-5.55	1.39	1.46
1	M	264	ARG	C-N	-5.54	1.24	1.33
2	P	407	TRP	N-CA	-5.52	1.39	1.46
2	R	407	TRP	N-CA	-5.51	1.39	1.46
2	L	280	SER	CA-C	-5.50	1.45	1.52
1	O	349	THR	N-CA	-5.50	1.39	1.46
2	H	407	TRP	N-CA	-5.50	1.39	1.46
2	D	407	TRP	N-CA	-5.49	1.39	1.46
2	F	407	TRP	N-CA	-5.49	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	407	TRP	N-CA	-5.49	1.39	1.46
2	N	407	TRP	N-CA	-5.47	1.39	1.46
1	O	262	TYR	CA-C	-5.47	1.46	1.52
2	H	280	SER	CA-C	-5.46	1.45	1.52
2	B	280	SER	CA-C	-5.46	1.45	1.52
2	L	407	TRP	N-CA	-5.46	1.39	1.46
2	J	280	SER	CA-C	-5.46	1.45	1.52
2	R	280	SER	CA-C	-5.45	1.45	1.52
1	K	262	TYR	CA-C	-5.44	1.46	1.52
2	F	280	SER	CA-C	-5.43	1.45	1.52
2	P	280	SER	CA-C	-5.43	1.45	1.52
2	J	407	TRP	N-CA	-5.42	1.39	1.46
1	I	262	TYR	CA-C	-5.42	1.46	1.52
1	E	262	TYR	CA-C	-5.41	1.46	1.52
2	D	280	SER	CA-C	-5.41	1.45	1.52
2	N	280	SER	CA-C	-5.41	1.45	1.52
1	A	262	TYR	CA-C	-5.39	1.46	1.52
1	G	262	TYR	CA-C	-5.39	1.46	1.52
1	C	262	TYR	CA-C	-5.38	1.46	1.52
1	Q	262	TYR	CA-C	-5.37	1.46	1.52
1	Q	49	PHE	N-CA	-5.36	1.36	1.46
1	K	49	PHE	N-CA	-5.36	1.36	1.46
1	E	35	GLN	CA-C	-5.35	1.45	1.52
1	M	262	TYR	CA-C	-5.35	1.46	1.52
1	I	36	MET	CA-C	-5.35	1.47	1.52
2	P	181	VAL	CA-CB	-5.35	1.46	1.54
1	E	49	PHE	N-CA	-5.34	1.36	1.46
1	M	49	PHE	N-CA	-5.33	1.36	1.46
1	E	36	MET	CA-C	-5.33	1.47	1.52
2	R	181	VAL	CA-CB	-5.32	1.46	1.54
1	O	49	PHE	N-CA	-5.32	1.36	1.46
1	A	49	PHE	N-CA	-5.32	1.36	1.46
2	D	181	VAL	CA-CB	-5.31	1.47	1.54
1	G	60	LYS	CA-C	-5.31	1.46	1.52
1	Q	36	MET	CA-C	-5.31	1.47	1.52
1	O	35	GLN	CA-C	-5.31	1.45	1.52
1	G	49	PHE	N-CA	-5.31	1.36	1.46
1	C	49	PHE	N-CA	-5.30	1.36	1.46
2	N	181	VAL	CA-CB	-5.30	1.47	1.54
2	B	181	VAL	CA-CB	-5.30	1.47	1.54
1	M	36	MET	CA-C	-5.30	1.47	1.52
1	G	35	GLN	CA-C	-5.29	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	181	VAL	CA-CB	-5.29	1.47	1.54
2	N	37	HIS	CA-C	-5.29	1.46	1.53
2	F	181	VAL	CA-CB	-5.29	1.47	1.54
1	O	36	MET	CA-C	-5.29	1.47	1.52
1	A	36	MET	CA-C	-5.28	1.47	1.52
1	A	35	GLN	CA-C	-5.28	1.45	1.52
1	I	35	GLN	CA-C	-5.28	1.45	1.52
1	C	35	GLN	CA-C	-5.28	1.45	1.52
1	O	60	LYS	CA-C	-5.27	1.46	1.52
1	C	60	LYS	CA-C	-5.27	1.46	1.52
2	R	112	ALA	N-CA	-5.27	1.39	1.46
1	C	36	MET	CA-C	-5.27	1.47	1.52
1	G	36	MET	CA-C	-5.27	1.47	1.52
1	I	49	PHE	N-CA	-5.27	1.36	1.46
1	M	35	GLN	CA-C	-5.27	1.45	1.52
2	L	112	ALA	N-CA	-5.26	1.39	1.46
2	H	37	HIS	CA-C	-5.26	1.46	1.53
2	L	181	VAL	CA-CB	-5.26	1.47	1.54
2	P	37	HIS	CA-C	-5.26	1.46	1.53
1	K	36	MET	CA-C	-5.26	1.47	1.52
2	H	112	ALA	N-CA	-5.25	1.39	1.46
2	B	112	ALA	N-CA	-5.25	1.39	1.46
1	Q	35	GLN	CA-C	-5.25	1.45	1.52
1	I	60	LYS	CA-C	-5.25	1.46	1.52
2	J	181	VAL	CA-CB	-5.25	1.47	1.54
2	L	37	HIS	CA-C	-5.24	1.46	1.53
2	D	112	ALA	N-CA	-5.24	1.39	1.46
2	J	112	ALA	N-CA	-5.23	1.39	1.46
1	M	60	LYS	CA-C	-5.23	1.46	1.52
1	E	60	LYS	CA-C	-5.23	1.46	1.52
1	A	60	LYS	CA-C	-5.23	1.46	1.52
2	B	37	HIS	CA-C	-5.23	1.46	1.53
2	F	112	ALA	N-CA	-5.23	1.39	1.46
2	N	112	ALA	N-CA	-5.23	1.39	1.46
2	R	37	HIS	CA-C	-5.23	1.46	1.53
1	K	60	LYS	CA-C	-5.22	1.46	1.52
2	D	37	HIS	CA-C	-5.20	1.46	1.53
2	J	37	HIS	CA-C	-5.20	1.46	1.53
1	K	35	GLN	CA-C	-5.20	1.45	1.52
1	Q	60	LYS	CA-C	-5.20	1.46	1.52
2	F	37	HIS	CA-C	-5.19	1.46	1.53
2	P	112	ALA	N-CA	-5.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	99	ALA	CA-C	-5.10	1.46	1.52
2	H	99	ALA	CA-C	-5.07	1.46	1.52
1	K	98	ASP	N-CA	-5.06	1.39	1.45
2	N	99	ALA	CA-C	-5.06	1.46	1.52
1	G	98	ASP	N-CA	-5.06	1.39	1.45
2	P	99	ALA	CA-C	-5.06	1.46	1.52
2	B	99	ALA	CA-C	-5.06	1.46	1.52
1	C	98	ASP	N-CA	-5.06	1.39	1.45
2	R	99	ALA	CA-C	-5.06	1.46	1.52
2	D	99	ALA	CA-C	-5.05	1.46	1.52
1	E	98	ASP	N-CA	-5.05	1.39	1.45
2	F	99	ALA	CA-C	-5.04	1.46	1.52
1	O	98	ASP	N-CA	-5.03	1.39	1.45
1	A	98	ASP	N-CA	-5.03	1.39	1.45
1	Q	98	ASP	N-CA	-5.03	1.39	1.45
1	M	102	ASN	N-CA	-5.02	1.40	1.46
1	C	99	ALA	CA-C	-5.02	1.45	1.52
1	I	99	ALA	CA-C	-5.02	1.45	1.52
2	L	99	ALA	CA-C	-5.01	1.46	1.52
1	O	99	ALA	CA-C	-5.01	1.45	1.52
1	G	346	TRP	C-N	-5.00	1.27	1.33
1	M	98	ASP	N-CA	-5.00	1.39	1.45

All (1575) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	264	ARG	CA-C-N	-18.83	101.49	121.45
1	G	264	ARG	C-N-CA	-18.83	101.49	121.45
1	O	264	ARG	CA-C-N	-18.83	101.49	121.45
1	O	264	ARG	C-N-CA	-18.83	101.49	121.45
1	K	264	ARG	CA-C-N	-18.82	101.50	121.45
1	K	264	ARG	C-N-CA	-18.82	101.50	121.45
1	E	264	ARG	CA-C-N	-18.82	101.50	121.45
1	E	264	ARG	C-N-CA	-18.82	101.50	121.45
1	Q	264	ARG	CA-C-N	-18.82	101.50	121.45
1	Q	264	ARG	C-N-CA	-18.82	101.50	121.45
1	A	264	ARG	CA-C-N	-18.82	101.50	121.45
1	A	264	ARG	C-N-CA	-18.82	101.50	121.45
1	C	264	ARG	CA-C-N	-18.81	101.51	121.45
1	C	264	ARG	C-N-CA	-18.81	101.51	121.45
1	M	264	ARG	CA-C-N	-18.81	101.51	121.45
1	M	264	ARG	C-N-CA	-18.81	101.51	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	264	ARG	CA-C-N	-18.77	101.56	121.45
1	I	264	ARG	C-N-CA	-18.77	101.56	121.45
2	J	96	GLN	CA-C-N	-13.33	102.47	122.47
2	J	96	GLN	C-N-CA	-13.33	102.47	122.47
2	L	96	GLN	CA-C-N	-13.31	102.50	122.47
2	L	96	GLN	C-N-CA	-13.31	102.50	122.47
2	N	96	GLN	CA-C-N	-13.31	102.50	122.47
2	N	96	GLN	C-N-CA	-13.31	102.50	122.47
2	B	96	GLN	CA-C-N	-13.30	102.53	122.47
2	B	96	GLN	C-N-CA	-13.30	102.53	122.47
2	R	96	GLN	CA-C-N	-13.29	102.53	122.47
2	R	96	GLN	C-N-CA	-13.29	102.53	122.47
2	H	96	GLN	CA-C-N	-13.29	102.53	122.47
2	H	96	GLN	C-N-CA	-13.29	102.53	122.47
2	D	96	GLN	CA-C-N	-13.28	102.55	122.47
2	D	96	GLN	C-N-CA	-13.28	102.55	122.47
2	P	96	GLN	CA-C-N	-13.29	102.54	122.47
2	P	96	GLN	C-N-CA	-13.29	102.54	122.47
2	F	96	GLN	CA-C-N	-13.28	102.55	122.47
2	F	96	GLN	C-N-CA	-13.28	102.55	122.47
2	D	101	ASN	CA-CB-CG	-11.53	101.07	112.60
2	P	101	ASN	CA-CB-CG	-11.52	101.08	112.60
2	J	101	ASN	CA-CB-CG	-11.51	101.09	112.60
2	N	101	ASN	CA-CB-CG	-11.51	101.09	112.60
2	L	101	ASN	CA-CB-CG	-11.50	101.10	112.60
2	B	101	ASN	CA-CB-CG	-11.50	101.10	112.60
2	H	101	ASN	CA-CB-CG	-11.49	101.11	112.60
2	R	101	ASN	CA-CB-CG	-11.48	101.12	112.60
2	F	101	ASN	CA-CB-CG	-11.48	101.12	112.60
1	O	142	GLY	CA-C-N	-10.72	109.18	121.83
1	O	142	GLY	C-N-CA	-10.72	109.18	121.83
1	A	142	GLY	CA-C-N	-10.69	109.21	121.83
1	A	142	GLY	C-N-CA	-10.69	109.21	121.83
1	I	142	GLY	CA-C-N	-10.69	109.22	121.83
1	I	142	GLY	C-N-CA	-10.69	109.22	121.83
1	C	142	GLY	CA-C-N	-10.68	109.23	121.83
1	C	142	GLY	C-N-CA	-10.68	109.23	121.83
1	M	142	GLY	CA-C-N	-10.68	109.23	121.83
1	M	142	GLY	C-N-CA	-10.68	109.23	121.83
1	G	142	GLY	CA-C-N	-10.67	109.24	121.83
1	G	142	GLY	C-N-CA	-10.67	109.24	121.83
1	Q	142	GLY	CA-C-N	-10.66	109.25	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	142	GLY	C-N-CA	-10.66	109.25	121.83
1	E	142	GLY	CA-C-N	-10.66	109.25	121.83
1	E	142	GLY	C-N-CA	-10.66	109.25	121.83
1	K	142	GLY	CA-C-N	-10.66	109.25	121.83
1	K	142	GLY	C-N-CA	-10.66	109.25	121.83
1	C	11	GLN	CB-CA-C	-10.45	94.48	110.88
1	Q	11	GLN	CB-CA-C	-10.44	94.50	110.88
1	K	11	GLN	CB-CA-C	-10.43	94.51	110.88
1	E	11	GLN	CB-CA-C	-10.43	94.51	110.88
1	A	11	GLN	CB-CA-C	-10.42	94.52	110.88
1	I	11	GLN	CB-CA-C	-10.42	94.53	110.88
1	O	11	GLN	CB-CA-C	-10.42	94.53	110.88
1	G	11	GLN	CB-CA-C	-10.41	94.53	110.88
1	M	11	GLN	CB-CA-C	-10.41	94.53	110.88
1	M	244	PHE	CA-CB-CG	-10.29	103.51	113.80
1	C	244	PHE	CA-CB-CG	-10.28	103.52	113.80
1	E	244	PHE	CA-CB-CG	-10.27	103.53	113.80
1	O	244	PHE	CA-CB-CG	-10.25	103.55	113.80
1	I	244	PHE	CA-CB-CG	-10.24	103.56	113.80
1	Q	244	PHE	CA-CB-CG	-10.24	103.56	113.80
1	A	244	PHE	CA-CB-CG	-10.24	103.56	113.80
1	G	244	PHE	CA-CB-CG	-10.22	103.58	113.80
1	K	244	PHE	CA-CB-CG	-10.22	103.58	113.80
1	K	265	GLY	CA-C-N	-10.11	106.93	122.81
1	K	265	GLY	C-N-CA	-10.11	106.93	122.81
1	I	265	GLY	CA-C-N	-10.11	106.94	122.81
1	I	265	GLY	C-N-CA	-10.11	106.94	122.81
1	O	265	GLY	CA-C-N	-10.11	106.94	122.81
1	O	265	GLY	C-N-CA	-10.11	106.94	122.81
1	C	265	GLY	CA-C-N	-10.10	106.95	122.81
1	C	265	GLY	C-N-CA	-10.10	106.95	122.81
1	A	265	GLY	CA-C-N	-10.10	106.95	122.81
1	A	265	GLY	C-N-CA	-10.10	106.95	122.81
1	M	265	GLY	CA-C-N	-10.10	106.96	122.81
1	M	265	GLY	C-N-CA	-10.10	106.96	122.81
1	G	265	GLY	CA-C-N	-10.10	106.96	122.81
1	G	265	GLY	C-N-CA	-10.10	106.96	122.81
1	E	265	GLY	CA-C-N	-10.08	106.98	122.81
1	E	265	GLY	C-N-CA	-10.08	106.98	122.81
1	Q	265	GLY	CA-C-N	-10.07	106.99	122.81
1	Q	265	GLY	C-N-CA	-10.07	106.99	122.81
1	O	265	GLY	O-C-N	10.02	137.23	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	GLY	O-C-N	9.99	137.19	123.11
1	K	265	GLY	O-C-N	9.99	137.19	123.11
1	M	265	GLY	O-C-N	9.98	137.19	123.11
1	C	265	GLY	O-C-N	9.98	137.18	123.11
1	G	265	GLY	O-C-N	9.98	137.18	123.11
1	I	265	GLY	O-C-N	9.97	137.17	123.11
1	E	265	GLY	O-C-N	9.95	137.14	123.11
1	Q	265	GLY	O-C-N	9.95	137.14	123.11
1	I	73	THR	N-CA-C	9.73	122.78	111.11
1	M	73	THR	N-CA-C	9.72	122.77	111.11
1	C	73	THR	N-CA-C	9.72	122.77	111.11
1	K	73	THR	N-CA-C	9.72	122.77	111.11
1	A	73	THR	N-CA-C	9.71	122.76	111.11
1	O	73	THR	N-CA-C	9.70	122.75	111.11
1	G	73	THR	N-CA-C	9.70	122.75	111.11
1	Q	73	THR	N-CA-C	9.69	122.74	111.11
1	E	73	THR	N-CA-C	9.68	122.73	111.11
2	D	378	ILE	CA-C-N	-9.33	114.42	121.61
2	D	378	ILE	C-N-CA	-9.33	114.42	121.61
2	H	378	ILE	CA-C-N	-9.32	114.43	121.61
2	H	378	ILE	C-N-CA	-9.32	114.43	121.61
2	N	378	ILE	CA-C-N	-9.28	114.47	121.61
2	N	378	ILE	C-N-CA	-9.28	114.47	121.61
2	B	378	ILE	CA-C-N	-9.27	114.47	121.61
2	B	378	ILE	C-N-CA	-9.27	114.47	121.61
2	L	378	ILE	CA-C-N	-9.26	114.48	121.61
2	L	378	ILE	C-N-CA	-9.26	114.48	121.61
2	R	378	ILE	CA-C-N	-9.26	114.48	121.61
2	R	378	ILE	C-N-CA	-9.26	114.48	121.61
2	F	378	ILE	CA-C-N	-9.25	114.49	121.61
2	F	378	ILE	C-N-CA	-9.25	114.49	121.61
2	P	378	ILE	CA-C-N	-9.25	114.49	121.61
2	P	378	ILE	C-N-CA	-9.25	114.49	121.61
2	J	378	ILE	CA-C-N	-9.21	114.52	121.61
2	J	378	ILE	C-N-CA	-9.21	114.52	121.61
2	P	101	ASN	CB-CG-ND2	9.13	130.10	116.40
2	B	101	ASN	CB-CG-ND2	9.12	130.07	116.40
2	H	101	ASN	CB-CG-ND2	9.12	130.07	116.40
2	J	101	ASN	CB-CG-ND2	9.12	130.07	116.40
2	F	101	ASN	CB-CG-ND2	9.11	130.06	116.40
2	N	101	ASN	CB-CG-ND2	9.11	130.06	116.40
2	D	101	ASN	CB-CG-ND2	9.11	130.06	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	101	ASN	CB-CG-ND2	9.11	130.06	116.40
2	L	101	ASN	CB-CG-ND2	9.09	130.04	116.40
1	Q	98	ASP	N-CA-C	9.04	123.90	110.52
1	G	98	ASP	N-CA-C	9.02	123.87	110.52
1	E	98	ASP	N-CA-C	9.02	123.87	110.52
1	A	98	ASP	N-CA-C	9.01	123.86	110.52
1	K	98	ASP	N-CA-C	9.01	123.85	110.52
1	M	98	ASP	N-CA-C	9.01	123.85	110.52
1	I	98	ASP	N-CA-C	9.00	123.84	110.52
2	R	48	ARG	NE-CZ-NH1	9.00	130.50	121.50
1	O	98	ASP	N-CA-C	9.00	123.83	110.52
1	C	98	ASP	N-CA-C	8.98	123.81	110.52
2	P	48	ARG	NE-CZ-NH1	8.96	130.46	121.50
2	J	48	ARG	NE-CZ-NH1	8.95	130.45	121.50
2	H	48	ARG	NE-CZ-NH1	8.95	130.45	121.50
2	B	48	ARG	NE-CZ-NH1	8.94	130.44	121.50
2	L	48	ARG	NE-CZ-NH1	8.93	130.43	121.50
2	N	48	ARG	NE-CZ-NH1	8.93	130.43	121.50
2	D	48	ARG	NE-CZ-NH1	8.93	130.43	121.50
2	F	48	ARG	NE-CZ-NH1	8.90	130.40	121.50
1	M	228	ASN	CA-CB-CG	-8.72	103.88	112.60
1	C	228	ASN	CA-CB-CG	-8.71	103.89	112.60
1	O	228	ASN	CA-CB-CG	-8.71	103.89	112.60
1	G	228	ASN	CA-CB-CG	-8.69	103.91	112.60
1	I	228	ASN	CA-CB-CG	-8.69	103.91	112.60
1	A	228	ASN	CA-CB-CG	-8.69	103.91	112.60
1	E	228	ASN	CA-CB-CG	-8.67	103.93	112.60
1	Q	228	ASN	CA-CB-CG	-8.67	103.93	112.60
1	K	228	ASN	CA-CB-CG	-8.65	103.95	112.60
2	N	96	GLN	N-CA-C	8.60	124.46	113.88
2	F	96	GLN	N-CA-C	8.59	124.45	113.88
1	I	347	CYS	N-CA-C	8.59	125.01	108.85
1	K	347	CYS	N-CA-C	8.59	124.99	108.85
1	O	347	CYS	N-CA-C	8.58	124.98	108.85
1	A	347	CYS	N-CA-C	8.57	124.96	108.85
1	Q	347	CYS	N-CA-C	8.56	124.95	108.85
1	C	347	CYS	N-CA-C	8.56	124.94	108.85
1	E	347	CYS	N-CA-C	8.56	124.94	108.85
2	L	400	ARG	NE-CZ-NH2	8.56	126.90	119.20
1	G	347	CYS	N-CA-C	8.55	124.93	108.85
2	H	400	ARG	NE-CZ-NH2	8.55	126.89	119.20
2	F	400	ARG	NE-CZ-NH2	8.53	126.88	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	347	CYS	N-CA-C	8.53	124.89	108.85
2	J	400	ARG	NE-CZ-NH2	8.51	126.86	119.20
2	B	400	ARG	NE-CZ-NH2	8.50	126.85	119.20
2	N	400	ARG	NE-CZ-NH2	8.49	126.85	119.20
2	P	400	ARG	NE-CZ-NH2	8.45	126.81	119.20
2	R	400	ARG	NE-CZ-NH2	8.45	126.81	119.20
2	D	400	ARG	NE-CZ-NH2	8.44	126.80	119.20
2	P	308	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	G	438	ASP	CA-C-N	-8.38	106.61	121.70
1	G	438	ASP	C-N-CA	-8.38	106.61	121.70
1	M	438	ASP	CA-C-N	-8.38	106.61	121.70
1	M	438	ASP	C-N-CA	-8.38	106.61	121.70
1	O	438	ASP	CA-C-N	-8.38	106.62	121.70
1	O	438	ASP	C-N-CA	-8.38	106.62	121.70
1	A	438	ASP	CA-C-N	-8.37	106.64	121.70
1	A	438	ASP	C-N-CA	-8.37	106.64	121.70
1	C	438	ASP	CA-C-N	-8.37	106.64	121.70
1	C	438	ASP	C-N-CA	-8.37	106.64	121.70
1	Q	438	ASP	CA-C-N	-8.37	106.64	121.70
1	Q	438	ASP	C-N-CA	-8.37	106.64	121.70
2	F	308	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	I	438	ASP	CA-C-N	-8.36	106.65	121.70
1	I	438	ASP	C-N-CA	-8.36	106.65	121.70
2	J	308	ARG	NE-CZ-NH2	-8.36	111.68	119.20
1	E	438	ASP	CA-C-N	-8.35	106.67	121.70
1	E	438	ASP	C-N-CA	-8.35	106.67	121.70
1	K	438	ASP	CA-C-N	-8.35	106.68	121.70
1	K	438	ASP	C-N-CA	-8.35	106.68	121.70
2	L	308	ARG	NE-CZ-NH2	-8.34	111.70	119.20
2	B	308	ARG	NE-CZ-NH2	-8.32	111.71	119.20
2	R	308	ARG	NE-CZ-NH2	-8.31	111.72	119.20
2	D	308	ARG	NE-CZ-NH2	-8.31	111.72	119.20
2	H	308	ARG	NE-CZ-NH2	-8.27	111.75	119.20
2	N	308	ARG	NE-CZ-NH2	-8.27	111.75	119.20
1	C	266	HIS	CA-CB-CG	-8.27	105.53	113.80
1	E	266	HIS	CA-CB-CG	-8.26	105.54	113.80
1	O	266	HIS	CA-CB-CG	-8.25	105.55	113.80
1	A	266	HIS	CA-CB-CG	-8.24	105.56	113.80
2	D	96	GLN	N-CA-C	8.23	124.51	113.97
1	I	266	HIS	CA-CB-CG	-8.23	105.57	113.80
2	L	96	GLN	N-CA-C	8.23	124.51	113.97
1	M	266	HIS	CA-CB-CG	-8.23	105.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	266	HIS	CA-CB-CG	-8.23	105.57	113.80
1	G	266	HIS	CA-CB-CG	-8.22	105.58	113.80
2	J	96	GLN	N-CA-C	8.22	124.50	113.97
1	K	266	HIS	CA-CB-CG	-8.22	105.58	113.80
2	P	96	GLN	N-CA-C	8.21	124.48	113.97
2	R	96	GLN	N-CA-C	8.21	124.48	113.97
2	H	96	GLN	N-CA-C	8.21	124.48	113.97
2	B	96	GLN	N-CA-C	8.21	124.47	113.97
1	M	190	THR	CB-CA-C	-8.08	95.16	110.67
1	K	190	THR	CB-CA-C	-8.07	95.18	110.67
1	O	190	THR	CB-CA-C	-8.06	95.19	110.67
1	I	190	THR	CB-CA-C	-8.06	95.19	110.67
1	A	190	THR	CB-CA-C	-8.06	95.20	110.67
1	E	190	THR	CB-CA-C	-8.06	95.20	110.67
1	Q	190	THR	CB-CA-C	-8.06	95.20	110.67
1	G	190	THR	CB-CA-C	-8.06	95.20	110.67
1	C	190	THR	CB-CA-C	-8.04	95.23	110.67
1	O	11	GLN	N-CA-CB	7.99	121.59	110.01
1	G	11	GLN	N-CA-CB	7.98	121.58	110.01
1	I	11	GLN	N-CA-CB	7.98	121.58	110.01
1	A	11	GLN	N-CA-CB	7.97	121.56	110.01
1	C	11	GLN	N-CA-CB	7.96	121.56	110.01
1	Q	11	GLN	N-CA-CB	7.96	121.55	110.01
1	E	11	GLN	N-CA-CB	7.95	121.54	110.01
1	G	176	GLN	CA-C-N	-7.95	112.52	123.10
1	G	176	GLN	C-N-CA	-7.95	112.52	123.10
1	K	11	GLN	N-CA-CB	7.95	121.54	110.01
1	K	176	GLN	CA-C-N	-7.94	112.54	123.10
1	K	176	GLN	C-N-CA	-7.94	112.54	123.10
1	M	11	GLN	N-CA-CB	7.94	121.52	110.01
1	I	176	GLN	CA-C-N	-7.92	112.56	123.10
1	I	176	GLN	C-N-CA	-7.92	112.56	123.10
1	E	176	GLN	CA-C-N	-7.92	112.57	123.10
1	E	176	GLN	C-N-CA	-7.92	112.57	123.10
1	M	176	GLN	CA-C-N	-7.92	112.57	123.10
1	M	176	GLN	C-N-CA	-7.92	112.57	123.10
1	A	176	GLN	CA-C-N	-7.92	112.57	123.10
1	A	176	GLN	C-N-CA	-7.92	112.57	123.10
1	C	176	GLN	CA-C-N	-7.91	112.57	123.10
1	C	176	GLN	C-N-CA	-7.91	112.57	123.10
1	O	176	GLN	CA-C-N	-7.90	112.59	123.10
1	O	176	GLN	C-N-CA	-7.90	112.59	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	176	GLN	CA-C-N	-7.89	112.61	123.10
1	Q	176	GLN	C-N-CA	-7.89	112.61	123.10
2	D	222	PRO	N-CA-C	7.80	123.61	111.21
2	F	222	PRO	N-CA-C	7.79	123.59	111.21
2	R	76	ASP	CA-CB-CG	7.77	120.37	112.60
2	N	222	PRO	N-CA-C	7.77	123.56	111.21
2	J	222	PRO	N-CA-C	7.77	123.56	111.21
2	F	76	ASP	CA-CB-CG	7.76	120.36	112.60
2	P	76	ASP	CA-CB-CG	7.76	120.36	112.60
2	B	222	PRO	N-CA-C	7.76	123.55	111.21
2	R	222	PRO	N-CA-C	7.75	123.54	111.21
2	P	222	PRO	N-CA-C	7.75	123.53	111.21
2	L	222	PRO	N-CA-C	7.75	123.53	111.21
2	J	76	ASP	CA-CB-CG	7.75	120.35	112.60
2	H	222	PRO	N-CA-C	7.74	123.52	111.21
2	L	76	ASP	CA-CB-CG	7.74	120.34	112.60
1	G	438	ASP	O-C-N	7.74	131.99	122.86
2	B	76	ASP	CA-CB-CG	7.74	120.33	112.60
2	D	76	ASP	CA-CB-CG	7.73	120.33	112.60
1	M	438	ASP	O-C-N	7.73	131.98	122.86
1	A	438	ASP	O-C-N	7.72	131.97	122.86
1	C	438	ASP	O-C-N	7.72	131.97	122.86
1	I	438	ASP	O-C-N	7.71	131.96	122.86
1	O	438	ASP	O-C-N	7.71	131.95	122.86
2	H	76	ASP	CA-CB-CG	7.70	120.30	112.60
1	Q	438	ASP	O-C-N	7.70	131.95	122.86
2	N	76	ASP	CA-CB-CG	7.69	120.29	112.60
1	E	438	ASP	O-C-N	7.68	131.92	122.86
2	H	2	ARG	NE-CZ-NH1	7.67	129.17	121.50
2	B	139	HIS	N-CA-C	7.67	119.80	108.60
2	R	139	HIS	N-CA-C	7.67	119.80	108.60
2	D	139	HIS	N-CA-C	7.67	119.79	108.60
1	K	438	ASP	O-C-N	7.67	131.91	122.86
2	F	139	HIS	N-CA-C	7.66	119.79	108.60
2	J	139	HIS	N-CA-C	7.66	119.79	108.60
2	L	139	HIS	N-CA-C	7.66	119.79	108.60
2	N	139	HIS	N-CA-C	7.66	119.79	108.60
2	R	2	ARG	NE-CZ-NH1	7.66	129.16	121.50
2	H	139	HIS	N-CA-C	7.65	119.77	108.60
2	P	139	HIS	N-CA-C	7.65	119.77	108.60
1	E	49	PHE	CA-CB-CG	7.64	121.44	113.80
2	B	2	ARG	NE-CZ-NH1	7.64	129.14	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	49	PHE	CA-CB-CG	7.63	121.43	113.80
1	M	49	PHE	CA-CB-CG	7.63	121.43	113.80
1	Q	49	PHE	CA-CB-CG	7.62	121.42	113.80
1	G	49	PHE	CA-CB-CG	7.62	121.42	113.80
2	D	2	ARG	NE-CZ-NH1	7.61	129.11	121.50
2	L	2	ARG	NE-CZ-NH1	7.61	129.11	121.50
1	A	49	PHE	CA-CB-CG	7.61	121.41	113.80
2	F	2	ARG	NE-CZ-NH1	7.61	129.10	121.50
1	I	49	PHE	CA-CB-CG	7.60	121.40	113.80
2	N	2	ARG	NE-CZ-NH1	7.60	129.10	121.50
2	P	2	ARG	NE-CZ-NH1	7.60	129.10	121.50
1	C	49	PHE	CA-CB-CG	7.59	121.39	113.80
2	J	2	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	O	49	PHE	CA-CB-CG	7.59	121.39	113.80
1	G	120	ASP	CA-CB-CG	-7.56	105.04	112.60
1	Q	120	ASP	CA-CB-CG	-7.55	105.05	112.60
1	E	120	ASP	CA-CB-CG	-7.54	105.06	112.60
1	A	120	ASP	CA-CB-CG	-7.54	105.06	112.60
1	M	120	ASP	CA-CB-CG	-7.54	105.06	112.60
2	D	33	THR	CA-C-N	-7.53	114.64	123.08
2	D	33	THR	C-N-CA	-7.53	114.64	123.08
1	O	120	ASP	CA-CB-CG	-7.53	105.07	112.60
2	F	33	THR	CA-C-N	-7.51	114.67	123.08
2	F	33	THR	C-N-CA	-7.51	114.67	123.08
1	K	120	ASP	CA-CB-CG	-7.51	105.09	112.60
2	H	33	THR	CA-C-N	-7.51	114.67	123.08
2	H	33	THR	C-N-CA	-7.51	114.67	123.08
1	I	120	ASP	CA-CB-CG	-7.50	105.09	112.60
2	J	33	THR	CA-C-N	-7.50	114.68	123.08
2	J	33	THR	C-N-CA	-7.50	114.68	123.08
1	O	347	CYS	CA-C-N	-7.50	112.96	120.31
1	O	347	CYS	C-N-CA	-7.50	112.96	120.31
2	B	33	THR	CA-C-N	-7.50	114.68	123.08
2	B	33	THR	C-N-CA	-7.50	114.68	123.08
2	N	33	THR	CA-C-N	-7.50	114.68	123.08
2	N	33	THR	C-N-CA	-7.50	114.68	123.08
2	R	33	THR	CA-C-N	-7.50	114.68	123.08
2	R	33	THR	C-N-CA	-7.50	114.68	123.08
1	M	347	CYS	CA-C-N	-7.50	112.97	120.31
1	M	347	CYS	C-N-CA	-7.50	112.97	120.31
1	Q	347	CYS	CA-C-N	-7.50	112.97	120.31
1	Q	347	CYS	C-N-CA	-7.50	112.97	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	33	THR	CA-C-N	-7.49	114.69	123.08
2	P	33	THR	C-N-CA	-7.49	114.69	123.08
1	C	120	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	347	CYS	CA-C-N	-7.47	112.99	120.31
1	A	347	CYS	C-N-CA	-7.47	112.99	120.31
2	R	185	TYR	CB-CA-C	-7.47	98.14	110.85
2	F	185	TYR	CB-CA-C	-7.47	98.15	110.85
2	J	185	TYR	CB-CA-C	-7.47	98.15	110.85
2	D	185	TYR	CB-CA-C	-7.47	98.15	110.85
2	H	185	TYR	CB-CA-C	-7.47	98.16	110.85
2	L	185	TYR	CB-CA-C	-7.47	98.16	110.85
1	C	347	CYS	CA-C-N	-7.46	113.00	120.31
1	C	347	CYS	C-N-CA	-7.46	113.00	120.31
1	E	347	CYS	CA-C-N	-7.46	113.00	120.31
1	E	347	CYS	C-N-CA	-7.46	113.00	120.31
2	B	185	TYR	CB-CA-C	-7.46	98.18	110.85
2	L	33	THR	CA-C-N	-7.45	114.73	123.08
2	L	33	THR	C-N-CA	-7.45	114.73	123.08
1	G	347	CYS	CA-C-N	-7.45	113.01	120.31
1	G	347	CYS	C-N-CA	-7.45	113.01	120.31
1	K	347	CYS	CA-C-N	-7.44	113.02	120.31
1	K	347	CYS	C-N-CA	-7.44	113.02	120.31
2	P	185	TYR	CB-CA-C	-7.44	98.21	110.85
2	L	101	ASN	CB-CG-OD1	-7.42	105.95	120.80
1	G	50	ASN	CA-CB-CG	-7.42	105.18	112.60
1	I	50	ASN	CA-CB-CG	-7.42	105.18	112.60
2	N	185	TYR	CB-CA-C	-7.42	98.23	110.85
1	I	347	CYS	CA-C-N	-7.42	113.04	120.31
1	I	347	CYS	C-N-CA	-7.42	113.04	120.31
1	M	50	ASN	CA-CB-CG	-7.42	105.18	112.60
2	P	101	ASN	CB-CG-OD1	-7.41	105.98	120.80
2	D	101	ASN	CB-CG-OD1	-7.40	106.00	120.80
2	B	101	ASN	CB-CG-OD1	-7.40	106.00	120.80
1	A	50	ASN	CA-CB-CG	-7.40	105.20	112.60
2	F	101	ASN	CB-CG-OD1	-7.40	106.01	120.80
1	K	50	ASN	CA-CB-CG	-7.40	105.20	112.60
2	N	101	ASN	CB-CG-OD1	-7.39	106.01	120.80
1	O	50	ASN	CA-CB-CG	-7.39	105.21	112.60
2	F	177	VAL	N-CA-C	7.39	116.95	106.53
2	H	101	ASN	CB-CG-OD1	-7.39	106.02	120.80
2	R	177	VAL	N-CA-C	7.39	116.95	106.53
2	J	101	ASN	CB-CG-OD1	-7.39	106.02	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	177	VAL	N-CA-C	7.39	116.95	106.53
2	L	88	ARG	NE-CZ-NH1	7.39	128.89	121.50
2	D	177	VAL	N-CA-C	7.38	116.94	106.53
2	R	101	ASN	CB-CG-OD1	-7.38	106.03	120.80
1	E	50	ASN	CA-CB-CG	-7.38	105.22	112.60
1	Q	50	ASN	CA-CB-CG	-7.38	105.22	112.60
2	P	177	VAL	N-CA-C	7.38	116.94	106.53
2	L	177	VAL	N-CA-C	7.38	116.93	106.53
2	N	177	VAL	N-CA-C	7.38	116.93	106.53
2	H	177	VAL	N-CA-C	7.37	116.92	106.53
2	B	177	VAL	N-CA-C	7.37	116.92	106.53
1	C	50	ASN	CA-CB-CG	-7.36	105.24	112.60
2	N	88	ARG	NE-CZ-NH1	7.34	128.84	121.50
2	J	88	ARG	NE-CZ-NH1	7.34	128.84	121.50
2	B	88	ARG	NE-CZ-NH1	7.33	128.82	121.50
2	D	88	ARG	NE-CZ-NH1	7.33	128.82	121.50
2	H	88	ARG	NE-CZ-NH1	7.32	128.81	121.50
2	R	88	ARG	NE-CZ-NH1	7.30	128.80	121.50
2	P	88	ARG	NE-CZ-NH1	7.29	128.79	121.50
1	Q	346	TRP	N-CA-C	7.29	121.27	112.38
1	E	346	TRP	N-CA-C	7.26	121.24	112.38
1	O	346	TRP	N-CA-C	7.26	121.24	112.38
2	F	88	ARG	NE-CZ-NH1	7.25	128.75	121.50
1	M	346	TRP	N-CA-C	7.25	121.23	112.38
1	A	346	TRP	N-CA-C	7.25	121.22	112.38
1	C	346	TRP	N-CA-C	7.23	121.20	112.38
1	I	346	TRP	N-CA-C	7.23	121.20	112.38
1	G	346	TRP	N-CA-C	7.22	121.19	112.38
1	K	346	TRP	N-CA-C	7.22	121.18	112.38
2	P	196	GLU	CB-CG-CD	7.16	124.77	112.60
2	D	196	GLU	CB-CG-CD	7.15	124.76	112.60
2	J	196	GLU	CB-CG-CD	7.15	124.76	112.60
2	R	196	GLU	CB-CG-CD	7.15	124.76	112.60
2	B	196	GLU	CB-CG-CD	7.14	124.74	112.60
2	H	196	GLU	CB-CG-CD	7.14	124.73	112.60
2	F	196	GLU	CB-CG-CD	7.13	124.73	112.60
2	N	196	GLU	CB-CG-CD	7.13	124.72	112.60
2	L	196	GLU	CB-CG-CD	7.12	124.70	112.60
1	C	28	HIS	CA-CB-CG	-7.11	106.69	113.80
1	I	28	HIS	CA-CB-CG	-7.08	106.72	113.80
1	O	28	HIS	CA-CB-CG	-7.08	106.72	113.80
1	A	28	HIS	CA-CB-CG	-7.07	106.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	28	HIS	CA-CB-CG	-7.07	106.73	113.80
1	E	28	HIS	CA-CB-CG	-7.07	106.73	113.80
1	M	28	HIS	CA-CB-CG	-7.04	106.75	113.80
1	G	28	HIS	CA-CB-CG	-7.04	106.76	113.80
1	K	28	HIS	CA-CB-CG	-7.04	106.76	113.80
2	R	251	ASP	CA-CB-CG	-6.99	105.61	112.60
2	P	251	ASP	CA-CB-CG	-6.98	105.62	112.60
2	J	251	ASP	CA-CB-CG	-6.97	105.63	112.60
2	F	251	ASP	CA-CB-CG	-6.97	105.63	112.60
2	H	251	ASP	CA-CB-CG	-6.97	105.63	112.60
2	L	251	ASP	CA-CB-CG	-6.97	105.63	112.60
2	N	251	ASP	CA-CB-CG	-6.96	105.64	112.60
1	C	36	MET	CG-SD-CE	6.96	116.21	100.90
1	E	36	MET	CG-SD-CE	6.96	116.20	100.90
2	D	251	ASP	CA-CB-CG	-6.95	105.65	112.60
1	M	36	MET	CG-SD-CE	6.95	116.19	100.90
2	B	251	ASP	CA-CB-CG	-6.95	105.65	112.60
1	I	36	MET	CG-SD-CE	6.95	116.19	100.90
1	Q	36	MET	CG-SD-CE	6.95	116.19	100.90
1	A	36	MET	CG-SD-CE	6.94	116.17	100.90
1	K	36	MET	CG-SD-CE	6.93	116.15	100.90
1	O	36	MET	CG-SD-CE	6.93	116.14	100.90
1	G	36	MET	CG-SD-CE	6.92	116.14	100.90
2	R	110	GLU	N-CA-C	6.83	120.09	111.69
2	D	110	GLU	N-CA-C	6.82	120.08	111.69
2	F	110	GLU	N-CA-C	6.82	120.08	111.69
2	H	110	GLU	N-CA-C	6.82	120.07	111.69
2	N	110	GLU	N-CA-C	6.82	120.07	111.69
2	B	110	GLU	N-CA-C	6.81	120.07	111.69
2	J	110	GLU	N-CA-C	6.80	120.06	111.69
2	L	110	GLU	N-CA-C	6.80	120.06	111.69
2	P	110	GLU	N-CA-C	6.80	120.05	111.69
2	R	48	ARG	NE-CZ-NH2	-6.78	113.10	119.20
2	J	427	ASP	CA-CB-CG	-6.77	105.83	112.60
2	P	427	ASP	CA-CB-CG	-6.75	105.86	112.60
2	L	48	ARG	NE-CZ-NH2	-6.74	113.13	119.20
2	J	48	ARG	NE-CZ-NH2	-6.74	113.13	119.20
2	B	48	ARG	NE-CZ-NH2	-6.74	113.14	119.20
2	H	194	LEU	N-CA-C	6.74	118.42	111.14
2	D	427	ASP	CA-CB-CG	-6.74	105.86	112.60
2	P	48	ARG	NE-CZ-NH2	-6.74	113.14	119.20
2	B	427	ASP	CA-CB-CG	-6.73	105.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	427	ASP	CA-CB-CG	-6.73	105.87	112.60
2	P	266	HIS	CA-CB-CG	-6.73	107.07	113.80
2	D	266	HIS	CA-CB-CG	-6.72	107.08	113.80
2	N	194	LEU	N-CA-C	6.72	118.39	111.14
2	B	266	HIS	CA-CB-CG	-6.72	107.08	113.80
2	F	266	HIS	CA-CB-CG	-6.72	107.08	113.80
2	N	48	ARG	NE-CZ-NH2	-6.72	113.16	119.20
2	B	194	LEU	N-CA-C	6.71	118.39	111.14
2	N	266	HIS	CA-CB-CG	-6.71	107.09	113.80
2	L	266	HIS	CA-CB-CG	-6.71	107.09	113.80
2	D	48	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	H	266	HIS	CA-CB-CG	-6.71	107.09	113.80
2	L	427	ASP	CA-CB-CG	-6.71	105.89	112.60
2	F	48	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	J	266	HIS	CA-CB-CG	-6.70	107.10	113.80
2	P	194	LEU	N-CA-C	6.70	118.38	111.14
2	H	427	ASP	CA-CB-CG	-6.70	105.90	112.60
2	L	194	LEU	N-CA-C	6.70	118.38	111.14
2	N	427	ASP	CA-CB-CG	-6.70	105.90	112.60
2	F	427	ASP	CA-CB-CG	-6.70	105.90	112.60
2	F	194	LEU	N-CA-C	6.69	118.37	111.14
2	R	266	HIS	CA-CB-CG	-6.69	107.11	113.80
2	H	48	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	R	194	LEU	N-CA-C	6.68	118.36	111.14
2	D	194	LEU	N-CA-C	6.68	118.36	111.14
2	J	194	LEU	N-CA-C	6.68	118.35	111.14
2	N	176	LYS	CA-C-N	-6.67	114.86	122.93
2	N	176	LYS	C-N-CA	-6.67	114.86	122.93
2	P	176	LYS	CA-C-N	-6.67	114.86	122.93
2	P	176	LYS	C-N-CA	-6.67	114.86	122.93
2	D	176	LYS	CA-C-N	-6.66	114.87	122.93
2	D	176	LYS	C-N-CA	-6.66	114.87	122.93
2	F	176	LYS	CA-C-N	-6.66	114.87	122.93
2	F	176	LYS	C-N-CA	-6.66	114.87	122.93
2	B	176	LYS	CA-C-N	-6.65	114.88	122.93
2	B	176	LYS	C-N-CA	-6.65	114.88	122.93
2	J	176	LYS	CA-C-N	-6.64	114.89	122.93
2	J	176	LYS	C-N-CA	-6.64	114.89	122.93
2	H	176	LYS	CA-C-N	-6.63	114.91	122.93
2	H	176	LYS	C-N-CA	-6.63	114.91	122.93
2	L	176	LYS	CA-C-N	-6.62	114.92	122.93
2	L	176	LYS	C-N-CA	-6.62	114.92	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	176	LYS	CA-C-N	-6.62	114.92	122.93
2	R	176	LYS	C-N-CA	-6.62	114.92	122.93
2	H	14	ASN	CA-CB-CG	-6.58	106.02	112.60
2	F	14	ASN	CA-CB-CG	-6.58	106.02	112.60
2	R	14	ASN	CA-CB-CG	-6.58	106.02	112.60
2	L	14	ASN	CA-CB-CG	-6.58	106.02	112.60
2	N	14	ASN	CA-CB-CG	-6.57	106.03	112.60
2	B	14	ASN	CA-CB-CG	-6.57	106.03	112.60
2	P	14	ASN	CA-CB-CG	-6.55	106.05	112.60
2	D	14	ASN	CA-CB-CG	-6.54	106.06	112.60
2	J	14	ASN	CA-CB-CG	-6.54	106.06	112.60
2	P	179	ASP	CA-CB-CG	6.53	119.13	112.60
2	J	179	ASP	CA-CB-CG	6.52	119.12	112.60
2	L	401	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	L	179	ASP	CA-CB-CG	6.51	119.11	112.60
2	F	401	ARG	NE-CZ-NH2	6.50	125.05	119.20
2	R	401	ARG	NE-CZ-NH2	6.50	125.05	119.20
2	J	401	ARG	NE-CZ-NH2	6.50	125.05	119.20
2	R	179	ASP	CA-CB-CG	6.49	119.09	112.60
2	B	179	ASP	CA-CB-CG	6.49	119.09	112.60
2	F	179	ASP	CA-CB-CG	6.48	119.08	112.60
2	D	179	ASP	CA-CB-CG	6.48	119.08	112.60
2	N	179	ASP	CA-CB-CG	6.47	119.07	112.60
2	B	401	ARG	NE-CZ-NH2	6.46	125.02	119.20
2	N	401	ARG	NE-CZ-NH2	6.46	125.02	119.20
2	H	179	ASP	CA-CB-CG	6.46	119.06	112.60
2	D	401	ARG	NE-CZ-NH2	6.46	125.01	119.20
2	H	401	ARG	NE-CZ-NH2	6.44	125.00	119.20
2	P	401	ARG	NE-CZ-NH2	6.43	124.98	119.20
2	N	88	ARG	NE-CZ-NH2	-6.40	113.44	119.20
2	L	88	ARG	NE-CZ-NH2	-6.38	113.46	119.20
2	H	88	ARG	NE-CZ-NH2	-6.35	113.49	119.20
2	J	88	ARG	NE-CZ-NH2	-6.35	113.49	119.20
2	B	88	ARG	NE-CZ-NH2	-6.34	113.49	119.20
2	R	88	ARG	NE-CZ-NH2	-6.33	113.50	119.20
2	R	34	GLY	N-CA-C	6.33	122.01	114.48
2	L	34	GLY	N-CA-C	6.33	122.01	114.48
2	H	34	GLY	N-CA-C	6.32	122.00	114.48
2	B	34	GLY	N-CA-C	6.32	122.00	114.48
2	D	240	THR	N-CA-C	6.32	120.25	112.54
2	P	34	GLY	N-CA-C	6.31	121.99	114.48
2	L	240	THR	N-CA-C	6.30	120.23	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	240	THR	N-CA-C	6.30	120.23	112.54
2	F	88	ARG	NE-CZ-NH2	-6.30	113.53	119.20
2	P	240	THR	N-CA-C	6.30	120.23	112.54
2	P	88	ARG	NE-CZ-NH2	-6.29	113.53	119.20
2	D	88	ARG	NE-CZ-NH2	-6.29	113.54	119.20
2	N	34	GLY	N-CA-C	6.29	121.97	114.48
1	O	353	VAL	CA-C-N	-6.29	116.88	122.73
1	O	353	VAL	C-N-CA	-6.29	116.88	122.73
2	R	240	THR	N-CA-C	6.29	120.22	112.54
2	D	34	GLY	N-CA-C	6.29	121.97	114.48
2	B	240	THR	N-CA-C	6.29	120.21	112.54
2	J	34	GLY	N-CA-C	6.29	121.96	114.48
2	H	240	THR	N-CA-C	6.28	120.20	112.54
1	I	353	VAL	CA-C-N	-6.28	116.89	122.73
1	I	353	VAL	C-N-CA	-6.28	116.89	122.73
1	C	353	VAL	CA-C-N	-6.28	116.89	122.73
1	C	353	VAL	C-N-CA	-6.28	116.89	122.73
2	F	240	THR	N-CA-C	6.28	120.20	112.54
2	J	240	THR	N-CA-C	6.27	120.19	112.54
1	Q	261	PRO	CA-C-N	-6.27	114.93	123.96
1	Q	261	PRO	C-N-CA	-6.27	114.93	123.96
1	Q	353	VAL	CA-C-N	-6.27	116.90	122.73
1	Q	353	VAL	C-N-CA	-6.27	116.90	122.73
1	A	261	PRO	CA-C-N	-6.27	114.93	123.96
1	A	261	PRO	C-N-CA	-6.27	114.93	123.96
1	A	353	VAL	CA-C-N	-6.27	116.90	122.73
1	A	353	VAL	C-N-CA	-6.27	116.90	122.73
2	F	34	GLY	N-CA-C	6.27	121.94	114.48
1	E	353	VAL	CA-C-N	-6.26	116.90	122.73
1	E	353	VAL	C-N-CA	-6.26	116.90	122.73
1	G	353	VAL	CA-C-N	-6.26	116.91	122.73
1	G	353	VAL	C-N-CA	-6.26	116.91	122.73
1	I	261	PRO	CA-C-N	-6.26	114.95	123.96
1	I	261	PRO	C-N-CA	-6.26	114.95	123.96
1	M	261	PRO	CA-C-N	-6.25	114.95	123.96
1	M	261	PRO	C-N-CA	-6.25	114.95	123.96
1	C	261	PRO	CA-C-N	-6.25	114.96	123.96
1	C	261	PRO	C-N-CA	-6.25	114.96	123.96
1	M	353	VAL	CA-C-N	-6.25	116.92	122.73
1	M	353	VAL	C-N-CA	-6.25	116.92	122.73
1	G	261	PRO	CA-C-N	-6.25	114.96	123.96
1	G	261	PRO	C-N-CA	-6.25	114.96	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	265	GLY	CA-C-O	6.24	129.40	121.53
1	K	353	VAL	CA-C-N	-6.24	116.93	122.73
1	K	353	VAL	C-N-CA	-6.24	116.93	122.73
1	K	265	GLY	CA-C-O	6.24	129.39	121.53
1	O	261	PRO	CA-C-N	-6.24	114.98	123.96
1	O	261	PRO	C-N-CA	-6.24	114.98	123.96
1	K	105	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	Q	265	GLY	CA-C-O	6.23	129.38	121.53
1	C	265	GLY	CA-C-O	6.22	129.37	121.53
1	K	261	PRO	CA-C-N	-6.22	115.00	123.96
1	K	261	PRO	C-N-CA	-6.22	115.00	123.96
1	A	265	GLY	CA-C-O	6.22	129.37	121.53
1	I	105	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	E	105	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	E	261	PRO	CA-C-N	-6.22	115.01	123.96
1	E	261	PRO	C-N-CA	-6.22	115.01	123.96
1	I	265	GLY	CA-C-O	6.21	129.36	121.53
1	M	265	GLY	CA-C-O	6.21	129.35	121.53
1	A	105	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	G	265	GLY	CA-C-O	6.21	129.35	121.53
1	M	105	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	O	105	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	O	265	GLY	CA-C-O	6.19	129.33	121.53
1	G	105	ARG	NE-CZ-NH2	-6.18	113.63	119.20
1	C	105	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	Q	105	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	E	177	VAL	N-CA-C	6.15	116.72	107.75
1	I	177	VAL	N-CA-C	6.14	116.71	107.75
1	M	177	VAL	N-CA-C	6.14	116.71	107.75
1	A	177	VAL	N-CA-C	6.14	116.71	107.75
1	Q	177	VAL	N-CA-C	6.13	116.70	107.75
1	I	53	PHE	N-CA-C	6.13	119.70	109.95
1	K	177	VAL	N-CA-C	6.13	116.70	107.75
1	C	177	VAL	N-CA-C	6.12	116.69	107.75
1	M	236	SER	CB-CA-C	-6.12	99.30	110.63
1	E	236	SER	CB-CA-C	-6.12	99.31	110.63
1	G	236	SER	CB-CA-C	-6.12	99.31	110.63
1	Q	53	PHE	N-CA-C	6.12	119.68	109.95
1	O	177	VAL	N-CA-C	6.12	116.68	107.75
1	A	53	PHE	N-CA-C	6.11	119.67	109.95
1	E	53	PHE	N-CA-C	6.11	119.67	109.95
1	K	53	PHE	N-CA-C	6.11	119.67	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	SER	CB-CA-C	-6.11	99.33	110.63
1	I	236	SER	CB-CA-C	-6.11	99.33	110.63
2	H	306	ASP	CA-CB-CG	-6.11	106.49	112.60
1	K	236	SER	CB-CA-C	-6.11	99.33	110.63
1	C	236	SER	CB-CA-C	-6.11	99.33	110.63
2	N	306	ASP	CA-CB-CG	-6.11	106.49	112.60
2	J	306	ASP	CA-CB-CG	-6.11	106.49	112.60
1	M	53	PHE	N-CA-C	6.10	119.65	109.95
1	Q	236	SER	CB-CA-C	-6.10	99.34	110.63
1	G	53	PHE	N-CA-C	6.10	119.65	109.95
1	G	177	VAL	N-CA-C	6.10	116.65	107.75
1	O	53	PHE	N-CA-C	6.10	119.64	109.95
1	O	236	SER	CB-CA-C	-6.10	99.35	110.63
2	B	306	ASP	CA-CB-CG	-6.09	106.51	112.60
1	C	53	PHE	N-CA-C	6.09	119.64	109.95
2	D	306	ASP	CA-CB-CG	-6.08	106.52	112.60
2	P	306	ASP	CA-CB-CG	-6.08	106.52	112.60
2	L	306	ASP	CA-CB-CG	-6.07	106.53	112.60
1	C	276	ILE	N-CA-C	6.07	116.86	108.12
2	R	306	ASP	CA-CB-CG	-6.06	106.54	112.60
2	F	306	ASP	CA-CB-CG	-6.05	106.55	112.60
1	E	276	ILE	N-CA-C	6.05	116.83	108.12
1	M	276	ILE	N-CA-C	6.04	116.82	108.12
1	G	276	ILE	N-CA-C	6.04	116.81	108.12
2	J	185	TYR	N-CA-CB	6.03	119.09	110.16
1	A	276	ILE	N-CA-C	6.03	116.81	108.12
1	O	276	ILE	N-CA-C	6.03	116.80	108.12
2	D	185	TYR	N-CA-CB	6.03	119.08	110.16
1	M	11	GLN	CA-CB-CG	6.03	126.15	114.10
2	L	185	TYR	N-CA-CB	6.02	119.07	110.16
1	Q	11	GLN	CA-CB-CG	6.02	126.14	114.10
2	B	185	TYR	N-CA-CB	6.02	119.07	110.16
1	I	276	ILE	N-CA-C	6.02	116.79	108.12
1	E	11	GLN	CA-CB-CG	6.02	126.14	114.10
1	A	11	GLN	CA-CB-CG	6.02	126.14	114.10
1	Q	276	ILE	N-CA-C	6.02	116.78	108.12
2	R	185	TYR	N-CA-CB	6.02	119.07	110.16
1	K	11	GLN	CA-CB-CG	6.02	126.13	114.10
1	O	11	GLN	CA-CB-CG	6.02	126.13	114.10
1	E	392	ASP	CA-CB-CG	-6.01	106.58	112.60
1	G	11	GLN	CA-CB-CG	6.01	126.13	114.10
2	N	185	TYR	N-CA-CB	6.01	119.06	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	GLN	CA-CB-CG	6.01	126.13	114.10
2	H	185	TYR	N-CA-CB	6.01	119.06	110.16
2	P	185	TYR	N-CA-CB	6.01	119.05	110.16
1	I	11	GLN	CA-CB-CG	6.01	126.12	114.10
2	F	185	TYR	N-CA-CB	6.00	119.03	110.16
2	F	404	PHE	CA-CB-CG	6.00	119.80	113.80
2	D	401	ARG	N-CA-C	5.99	120.59	113.28
2	R	267	PHE	CA-CB-CG	-5.99	107.81	113.80
2	F	401	ARG	N-CA-C	5.99	120.58	113.28
1	K	276	ILE	N-CA-C	5.99	116.74	108.12
1	C	392	ASP	CA-CB-CG	-5.97	106.63	112.60
2	R	404	PHE	CA-CB-CG	5.97	119.77	113.80
2	J	267	PHE	CA-CB-CG	-5.97	107.83	113.80
2	D	248	LEU	O-C-N	5.97	130.64	122.59
1	I	392	ASP	CA-CB-CG	-5.96	106.64	112.60
2	F	244	PHE	N-CA-C	5.96	118.21	110.40
2	H	267	PHE	CA-CB-CG	-5.96	107.84	113.80
2	L	244	PHE	N-CA-C	5.96	118.21	110.40
2	B	244	PHE	N-CA-C	5.96	118.21	110.40
2	P	248	LEU	O-C-N	5.96	130.64	122.59
2	N	267	PHE	CA-CB-CG	-5.96	107.84	113.80
2	B	248	LEU	O-C-N	5.96	130.63	122.59
2	D	404	PHE	CA-CB-CG	5.96	119.76	113.80
2	P	143	GLY	CA-C-N	5.96	126.59	119.98
2	P	143	GLY	C-N-CA	5.96	126.59	119.98
2	P	404	PHE	CA-CB-CG	5.96	119.76	113.80
2	R	248	LEU	O-C-N	5.96	130.63	122.59
2	H	404	PHE	CA-CB-CG	5.95	119.75	113.80
2	R	244	PHE	N-CA-C	5.95	118.20	110.40
2	B	404	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	392	ASP	CA-CB-CG	-5.95	106.65	112.60
2	D	244	PHE	N-CA-C	5.95	118.19	110.40
2	L	248	LEU	O-C-N	5.95	130.62	122.59
2	N	401	ARG	N-CA-C	5.95	120.54	113.28
1	Q	392	ASP	CA-CB-CG	-5.95	106.65	112.60
2	J	404	PHE	CA-CB-CG	5.95	119.75	113.80
2	P	401	ARG	N-CA-C	5.95	120.54	113.28
2	H	244	PHE	N-CA-C	5.95	118.19	110.40
1	M	392	ASP	CA-CB-CG	-5.95	106.66	112.60
2	B	267	PHE	CA-CB-CG	-5.94	107.86	113.80
2	J	244	PHE	N-CA-C	5.94	118.19	110.40
2	D	267	PHE	CA-CB-CG	-5.94	107.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	267	PHE	CA-CB-CG	-5.94	107.86	113.80
2	N	244	PHE	N-CA-C	5.94	118.18	110.40
2	B	401	ARG	N-CA-C	5.93	120.52	113.28
2	J	248	LEU	O-C-N	5.93	130.60	122.59
2	B	143	GLY	CA-C-N	5.93	126.56	119.98
2	B	143	GLY	C-N-CA	5.93	126.56	119.98
1	K	392	ASP	CA-CB-CG	-5.93	106.67	112.60
2	F	248	LEU	O-C-N	5.93	130.59	122.59
2	H	248	LEU	O-C-N	5.93	130.60	122.59
1	Q	102	ASN	CA-CB-CG	5.93	118.53	112.60
1	G	392	ASP	CA-CB-CG	-5.93	106.67	112.60
2	N	404	PHE	CA-CB-CG	5.93	119.73	113.80
2	L	267	PHE	CA-CB-CG	-5.92	107.88	113.80
2	L	404	PHE	CA-CB-CG	5.92	119.72	113.80
2	N	248	LEU	O-C-N	5.92	130.59	122.59
2	P	267	PHE	CA-CB-CG	-5.92	107.88	113.80
1	O	392	ASP	CA-CB-CG	-5.92	106.68	112.60
2	P	244	PHE	N-CA-C	5.92	118.15	110.40
2	D	143	GLY	CA-C-N	5.91	126.54	119.98
2	D	143	GLY	C-N-CA	5.91	126.54	119.98
2	L	143	GLY	CA-C-N	5.91	126.54	119.98
2	L	143	GLY	C-N-CA	5.91	126.54	119.98
1	O	102	ASN	CA-CB-CG	5.91	118.51	112.60
2	H	143	GLY	CA-C-N	5.91	126.54	119.98
2	H	143	GLY	C-N-CA	5.91	126.54	119.98
1	K	102	ASN	CA-CB-CG	5.91	118.51	112.60
1	I	102	ASN	CA-CB-CG	5.91	118.51	112.60
2	F	143	GLY	CA-C-N	5.91	126.54	119.98
2	F	143	GLY	C-N-CA	5.91	126.54	119.98
2	J	401	ARG	N-CA-C	5.91	120.49	113.28
2	N	143	GLY	CA-C-N	5.91	126.54	119.98
2	N	143	GLY	C-N-CA	5.91	126.54	119.98
1	M	102	ASN	CA-CB-CG	5.90	118.50	112.60
2	J	143	GLY	CA-C-N	5.90	126.53	119.98
2	J	143	GLY	C-N-CA	5.90	126.53	119.98
2	L	401	ARG	N-CA-C	5.90	120.48	113.28
1	E	102	ASN	CA-CB-CG	5.90	118.50	112.60
2	R	143	GLY	CA-C-N	5.90	126.53	119.98
2	R	143	GLY	C-N-CA	5.90	126.53	119.98
1	A	102	ASN	CA-CB-CG	5.89	118.49	112.60
1	G	102	ASN	CA-CB-CG	5.89	118.49	112.60
2	H	401	ARG	N-CA-C	5.89	120.46	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	61	TYR	CA-CB-CG	-5.88	103.31	113.90
1	Q	229	ARG	NE-CZ-NH2	5.88	124.49	119.20
2	R	216	THR	CB-CA-C	-5.87	99.52	109.03
2	N	61	TYR	CA-CB-CG	-5.87	103.33	113.90
1	K	229	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	J	408	TYR	N-CA-C	5.87	117.76	111.36
2	N	408	TYR	N-CA-C	5.87	117.76	111.36
1	C	102	ASN	CA-CB-CG	5.87	118.47	112.60
2	B	408	TYR	N-CA-C	5.87	117.75	111.36
2	H	61	TYR	CA-CB-CG	-5.87	103.34	113.90
2	P	408	TYR	N-CA-C	5.87	117.75	111.36
2	R	61	TYR	CA-CB-CG	-5.87	103.34	113.90
2	R	408	TYR	N-CA-C	5.87	117.75	111.36
2	H	216	THR	CB-CA-C	-5.86	99.53	109.03
1	I	229	ARG	NE-CZ-NH2	5.86	124.48	119.20
1	C	348	PRO	CA-N-CD	5.86	120.20	112.00
2	F	61	TYR	CA-CB-CG	-5.86	103.35	113.90
2	B	61	TYR	CA-CB-CG	-5.86	103.36	113.90
2	R	401	ARG	N-CA-C	5.86	120.49	113.23
1	C	357	TYR	N-CA-C	-5.86	105.23	112.90
1	Q	348	PRO	CA-N-CD	5.86	120.20	112.00
2	B	216	THR	CB-CA-C	-5.85	99.55	109.03
2	J	216	THR	CB-CA-C	-5.85	99.55	109.03
2	L	61	TYR	CA-CB-CG	-5.85	103.37	113.90
2	L	408	TYR	N-CA-C	5.85	117.74	111.36
2	P	268	PHE	CA-CB-CG	-5.85	107.95	113.80
2	L	216	THR	CB-CA-C	-5.85	99.56	109.03
1	Q	357	TYR	N-CA-C	-5.85	105.24	112.90
2	H	268	PHE	CA-CB-CG	-5.84	107.95	113.80
2	D	216	THR	CB-CA-C	-5.84	99.56	109.03
2	F	216	THR	CB-CA-C	-5.84	99.56	109.03
2	D	268	PHE	CA-CB-CG	-5.84	107.96	113.80
2	D	408	TYR	N-CA-C	5.84	117.73	111.36
1	I	357	TYR	N-CA-C	-5.84	105.25	112.90
2	J	61	TYR	CA-CB-CG	-5.84	103.38	113.90
2	N	216	THR	CB-CA-C	-5.84	99.57	109.03
1	A	229	ARG	NE-CZ-NH2	5.84	124.46	119.20
2	F	408	TYR	N-CA-C	5.84	117.73	111.36
2	J	106	GLY	N-CA-C	5.84	119.27	112.50
2	P	216	THR	CB-CA-C	-5.83	99.58	109.03
1	A	348	PRO	CA-N-CD	5.83	120.17	112.00
1	E	229	ARG	NE-CZ-NH2	5.83	124.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	408	TYR	N-CA-C	5.83	117.72	111.36
2	J	268	PHE	CA-CB-CG	-5.83	107.97	113.80
1	M	348	PRO	CA-N-CD	5.83	120.16	112.00
2	N	106	GLY	N-CA-C	5.83	119.27	112.50
1	O	357	TYR	N-CA-C	-5.83	105.26	112.90
2	R	268	PHE	CA-CB-CG	-5.83	107.97	113.80
2	N	268	PHE	CA-CB-CG	-5.83	107.97	113.80
2	P	61	TYR	CA-CB-CG	-5.83	103.41	113.90
2	B	106	GLY	N-CA-C	5.83	119.26	112.50
1	G	229	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	G	348	PRO	CA-N-CD	5.83	120.16	112.00
1	K	357	TYR	N-CA-C	-5.83	105.26	112.90
1	E	348	PRO	CA-N-CD	5.83	120.16	112.00
1	G	357	TYR	N-CA-C	-5.83	105.27	112.90
2	B	268	PHE	CA-CB-CG	-5.82	107.98	113.80
1	M	357	TYR	N-CA-C	-5.82	105.27	112.90
2	R	106	GLY	N-CA-C	5.82	119.25	112.50
1	A	357	TYR	N-CA-C	-5.82	105.28	112.90
1	I	348	PRO	CA-N-CD	5.82	120.15	112.00
1	O	348	PRO	CA-N-CD	5.82	120.14	112.00
1	C	229	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	O	229	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	M	229	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	F	106	GLY	N-CA-C	5.81	119.24	112.50
2	L	268	PHE	CA-CB-CG	-5.81	107.99	113.80
1	K	348	PRO	CA-N-CD	5.81	120.14	112.00
2	P	106	GLY	N-CA-C	5.81	119.24	112.50
1	E	357	TYR	N-CA-C	-5.80	105.30	112.90
2	F	268	PHE	CA-CB-CG	-5.80	108.00	113.80
2	D	106	GLY	N-CA-C	5.80	119.22	112.50
2	R	96	GLN	O-C-N	5.79	129.49	122.48
2	J	96	GLN	O-C-N	5.79	129.49	122.48
2	L	106	GLY	N-CA-C	5.79	119.22	112.50
2	H	106	GLY	N-CA-C	5.79	119.22	112.50
2	B	96	GLN	O-C-N	5.75	129.44	122.48
2	D	96	GLN	O-C-N	5.75	129.44	122.48
2	H	96	GLN	O-C-N	5.74	129.43	122.48
1	K	339	ARG	NE-CZ-NH2	5.74	124.37	119.20
2	F	268	PHE	N-CA-C	5.74	118.90	109.72
2	P	96	GLN	O-C-N	5.74	129.42	122.48
2	H	268	PHE	N-CA-C	5.74	118.90	109.72
2	L	268	PHE	N-CA-C	5.73	118.89	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	339	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	L	96	GLN	O-C-N	5.73	129.42	122.48
2	R	268	PHE	N-CA-C	5.73	118.89	109.72
1	G	339	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	B	268	PHE	N-CA-C	5.72	118.88	109.72
1	O	339	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	P	268	PHE	N-CA-C	5.72	118.88	109.72
2	N	268	PHE	N-CA-C	5.72	118.87	109.72
2	D	268	PHE	N-CA-C	5.72	118.86	109.72
2	J	268	PHE	N-CA-C	5.72	118.87	109.72
2	J	215	ARG	NE-CZ-NH2	-5.71	114.06	119.20
2	L	215	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	K	347	CYS	CB-CA-C	-5.70	102.49	110.13
1	A	339	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	C	339	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	R	215	ARG	NE-CZ-NH2	-5.70	114.08	119.20
1	E	339	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	E	347	CYS	CB-CA-C	-5.68	102.51	110.13
1	M	339	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	Q	339	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	M	347	CYS	CB-CA-C	-5.68	102.52	110.13
1	O	347	CYS	CB-CA-C	-5.67	102.53	110.13
2	B	215	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	A	347	CYS	CB-CA-C	-5.67	102.54	110.13
2	F	215	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	G	347	CYS	CB-CA-C	-5.66	102.54	110.13
1	K	337	THR	N-CA-C	5.66	120.32	113.41
1	C	347	CYS	CB-CA-C	-5.66	102.55	110.13
1	E	337	THR	N-CA-C	5.66	120.32	113.41
2	N	177	VAL	CB-CA-C	-5.66	105.02	111.59
1	E	356	ASN	CA-CB-CG	-5.66	106.94	112.60
2	P	215	ARG	NE-CZ-NH2	-5.66	114.11	119.20
2	H	215	ARG	NE-CZ-NH2	-5.66	114.11	119.20
2	P	177	VAL	CB-CA-C	-5.66	105.03	111.59
1	G	356	ASN	CA-CB-CG	-5.65	106.95	112.60
1	Q	347	CYS	CB-CA-C	-5.65	102.56	110.13
1	I	347	CYS	CB-CA-C	-5.65	102.56	110.13
1	I	337	THR	N-CA-C	5.65	120.30	113.41
1	A	337	THR	N-CA-C	5.64	120.29	113.41
1	O	356	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	337	THR	N-CA-C	5.64	120.29	113.41
2	L	177	VAL	CB-CA-C	-5.63	105.05	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	337	THR	N-CA-C	5.63	120.28	113.41
2	L	406	HIS	CA-C-N	-5.63	112.30	120.29
2	L	406	HIS	C-N-CA	-5.63	112.30	120.29
2	F	264	ARG	CA-C-N	-5.63	114.39	123.23
2	F	264	ARG	C-N-CA	-5.63	114.39	123.23
2	D	177	VAL	CB-CA-C	-5.62	105.06	111.59
2	H	264	ARG	CA-C-N	-5.62	114.40	123.23
2	H	264	ARG	C-N-CA	-5.62	114.40	123.23
2	J	406	HIS	CA-C-N	-5.62	112.30	120.29
2	J	406	HIS	C-N-CA	-5.62	112.30	120.29
1	O	337	THR	N-CA-C	5.62	120.27	113.41
2	F	177	VAL	CB-CA-C	-5.62	105.07	111.59
2	F	406	HIS	CA-C-N	-5.62	112.31	120.29
2	F	406	HIS	C-N-CA	-5.62	112.31	120.29
2	R	264	ARG	CA-C-N	-5.62	114.41	123.23
2	R	264	ARG	C-N-CA	-5.62	114.41	123.23
1	C	356	ASN	CA-CB-CG	-5.62	106.98	112.60
1	Q	356	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	356	ASN	CA-CB-CG	-5.62	106.98	112.60
2	D	264	ARG	CA-C-N	-5.62	114.41	123.23
2	D	264	ARG	C-N-CA	-5.62	114.41	123.23
1	G	349	THR	N-CA-C	5.62	122.76	110.80
1	Q	349	THR	N-CA-C	5.62	122.76	110.80
2	D	215	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	I	356	ASN	CA-CB-CG	-5.61	106.99	112.60
2	L	264	ARG	CA-C-N	-5.61	114.42	123.23
2	L	264	ARG	C-N-CA	-5.61	114.42	123.23
2	B	177	VAL	CB-CA-C	-5.61	105.08	111.59
2	B	406	HIS	CA-C-N	-5.61	112.32	120.29
2	B	406	HIS	C-N-CA	-5.61	112.32	120.29
1	G	337	THR	N-CA-C	5.61	120.25	113.41
2	H	406	HIS	CA-C-N	-5.61	112.33	120.29
2	H	406	HIS	C-N-CA	-5.61	112.33	120.29
2	J	264	ARG	CA-C-N	-5.61	114.43	123.23
2	J	264	ARG	C-N-CA	-5.61	114.43	123.23
1	K	356	ASN	CA-CB-CG	-5.61	106.99	112.60
2	J	177	VAL	CB-CA-C	-5.61	105.09	111.59
1	M	356	ASN	CA-CB-CG	-5.61	107.00	112.60
1	Q	337	THR	N-CA-C	5.61	120.25	113.41
2	N	406	HIS	CA-C-N	-5.60	112.33	120.29
2	N	406	HIS	C-N-CA	-5.60	112.33	120.29
2	B	264	ARG	CA-C-N	-5.60	114.43	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	264	ARG	C-N-CA	-5.60	114.43	123.23
2	N	215	ARG	NE-CZ-NH2	-5.60	114.16	119.20
2	R	406	HIS	CA-C-N	-5.60	112.34	120.29
2	R	406	HIS	C-N-CA	-5.60	112.34	120.29
1	E	349	THR	N-CA-C	5.60	122.73	110.80
1	A	349	THR	N-CA-C	5.60	122.72	110.80
2	H	176	LYS	N-CA-C	5.60	120.23	112.90
2	H	177	VAL	CB-CA-C	-5.60	105.10	111.59
1	K	349	THR	N-CA-C	5.60	122.72	110.80
2	L	424	ASN	CA-CB-CG	-5.60	107.00	112.60
1	M	349	THR	N-CA-C	5.60	122.72	110.80
2	N	243	ARG	N-CA-C	5.59	118.57	111.69
2	D	406	HIS	CA-C-N	-5.59	112.35	120.29
2	D	406	HIS	C-N-CA	-5.59	112.35	120.29
2	F	176	LYS	N-CA-C	5.59	120.22	112.90
2	R	176	LYS	N-CA-C	5.59	120.22	112.90
1	C	349	THR	N-CA-C	5.59	122.70	110.80
2	L	243	ARG	N-CA-C	5.59	118.56	111.69
2	P	406	HIS	CA-C-N	-5.59	112.35	120.29
2	P	406	HIS	C-N-CA	-5.59	112.35	120.29
1	K	200	CYS	CA-C-N	-5.59	115.11	122.99
1	K	200	CYS	C-N-CA	-5.59	115.11	122.99
2	B	176	LYS	N-CA-C	5.59	120.22	112.90
2	J	176	LYS	N-CA-C	5.59	120.22	112.90
1	Q	359	PRO	CA-C-N	5.59	125.49	119.85
1	Q	359	PRO	C-N-CA	5.59	125.49	119.85
1	I	349	THR	N-CA-C	5.58	122.70	110.80
2	J	424	ASN	CA-CB-CG	-5.58	107.02	112.60
1	O	349	THR	N-CA-C	5.58	122.69	110.80
2	L	176	LYS	N-CA-C	5.58	120.21	112.90
2	N	424	ASN	CA-CB-CG	-5.58	107.02	112.60
2	N	221	THR	N-CA-C	5.58	122.14	109.81
2	N	264	ARG	CA-C-N	-5.58	114.48	123.23
2	N	264	ARG	C-N-CA	-5.58	114.48	123.23
2	R	221	THR	N-CA-C	5.58	122.13	109.81
2	P	176	LYS	N-CA-C	5.57	120.20	112.90
2	R	243	ARG	N-CA-C	5.57	118.55	111.69
2	B	243	ARG	N-CA-C	5.57	118.54	111.69
2	P	243	ARG	N-CA-C	5.57	118.54	111.69
2	J	221	THR	N-CA-C	5.57	122.12	109.81
2	P	264	ARG	CA-C-N	-5.57	114.48	123.23
2	P	264	ARG	C-N-CA	-5.57	114.48	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	176	LYS	N-CA-C	5.57	120.19	112.90
2	N	176	LYS	N-CA-C	5.57	120.19	112.90
2	R	177	VAL	CB-CA-C	-5.57	105.13	111.59
2	B	424	ASN	CA-CB-CG	-5.57	107.03	112.60
2	J	243	ARG	N-CA-C	5.57	118.54	111.69
2	P	221	THR	N-CA-C	5.57	122.11	109.81
1	C	359	PRO	CA-C-N	5.56	125.47	119.85
1	C	359	PRO	C-N-CA	5.56	125.47	119.85
2	D	424	ASN	CA-CB-CG	-5.56	107.04	112.60
1	G	359	PRO	CA-C-N	5.56	125.47	119.85
1	G	359	PRO	C-N-CA	5.56	125.47	119.85
2	H	424	ASN	CA-CB-CG	-5.56	107.04	112.60
2	F	243	ARG	N-CA-C	5.56	118.53	111.69
2	B	221	THR	N-CA-C	5.56	122.10	109.81
1	C	200	CYS	CA-C-N	-5.56	115.15	122.99
1	C	200	CYS	C-N-CA	-5.56	115.15	122.99
2	D	221	THR	N-CA-C	5.56	122.10	109.81
2	F	424	ASN	CA-CB-CG	-5.56	107.04	112.60
1	M	200	CYS	CA-C-N	-5.56	115.15	122.99
1	M	200	CYS	C-N-CA	-5.56	115.15	122.99
2	R	60	LYS	CA-C-N	-5.56	115.15	122.99
2	R	60	LYS	C-N-CA	-5.56	115.15	122.99
1	G	200	CYS	CA-C-N	-5.56	115.16	122.99
1	G	200	CYS	C-N-CA	-5.56	115.16	122.99
1	K	359	PRO	CA-C-N	5.56	125.46	119.85
1	K	359	PRO	C-N-CA	5.56	125.46	119.85
2	H	243	ARG	N-CA-C	5.55	118.52	111.69
2	L	221	THR	N-CA-C	5.55	122.09	109.81
1	E	359	PRO	CA-C-N	5.55	125.46	119.85
1	E	359	PRO	C-N-CA	5.55	125.46	119.85
1	A	200	CYS	CA-C-N	-5.55	115.16	122.99
1	A	200	CYS	C-N-CA	-5.55	115.16	122.99
2	D	60	LYS	CA-C-N	-5.55	115.17	122.99
2	D	60	LYS	C-N-CA	-5.55	115.17	122.99
2	P	424	ASN	CA-CB-CG	-5.55	107.05	112.60
2	R	424	ASN	CA-CB-CG	-5.55	107.05	112.60
1	O	359	PRO	CA-C-N	5.55	125.45	119.85
1	O	359	PRO	C-N-CA	5.55	125.45	119.85
1	A	359	PRO	CA-C-N	5.54	125.45	119.85
1	A	359	PRO	C-N-CA	5.54	125.45	119.85
2	F	60	LYS	CA-C-N	-5.54	115.17	122.99
2	F	60	LYS	C-N-CA	-5.54	115.17	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	200	CYS	CA-C-N	-5.54	115.18	122.99
1	E	200	CYS	C-N-CA	-5.54	115.18	122.99
2	H	221	THR	N-CA-C	5.54	122.06	109.81
2	F	221	THR	N-CA-C	5.54	122.05	109.81
1	M	283	HIS	CA-CB-CG	-5.54	108.26	113.80
1	I	283	HIS	CA-CB-CG	-5.54	108.26	113.80
1	Q	283	HIS	CA-CB-CG	-5.54	108.26	113.80
2	B	60	LYS	CA-C-N	-5.53	115.19	122.99
2	B	60	LYS	C-N-CA	-5.53	115.19	122.99
1	G	354	GLY	CA-C-N	-5.53	115.47	123.11
1	G	354	GLY	C-N-CA	-5.53	115.47	123.11
1	I	359	PRO	CA-C-N	5.53	125.44	119.85
1	I	359	PRO	C-N-CA	5.53	125.44	119.85
2	J	60	LYS	CA-C-N	-5.53	115.19	122.99
2	J	60	LYS	C-N-CA	-5.53	115.19	122.99
1	I	200	CYS	CA-C-N	-5.53	115.19	122.99
1	I	200	CYS	C-N-CA	-5.53	115.19	122.99
1	Q	200	CYS	CA-C-N	-5.53	115.19	122.99
1	Q	200	CYS	C-N-CA	-5.53	115.19	122.99
2	H	60	LYS	CA-C-N	-5.53	115.19	122.99
2	H	60	LYS	C-N-CA	-5.53	115.19	122.99
1	I	309	HIS	CA-C-N	-5.53	116.80	122.27
1	I	309	HIS	C-N-CA	-5.53	116.80	122.27
1	O	283	HIS	CA-CB-CG	-5.53	108.27	113.80
2	L	60	LYS	CA-C-N	-5.53	115.20	122.99
2	L	60	LYS	C-N-CA	-5.53	115.20	122.99
1	M	359	PRO	CA-C-N	5.52	125.43	119.85
1	M	359	PRO	C-N-CA	5.52	125.43	119.85
1	E	283	HIS	CA-CB-CG	-5.52	108.28	113.80
1	E	345	ASP	N-CA-C	5.52	122.56	110.80
1	O	200	CYS	CA-C-N	-5.52	115.20	122.99
1	O	200	CYS	C-N-CA	-5.52	115.20	122.99
2	N	60	LYS	CA-C-N	-5.52	115.21	122.99
2	N	60	LYS	C-N-CA	-5.52	115.21	122.99
2	P	60	LYS	CA-C-N	-5.52	115.21	122.99
2	P	60	LYS	C-N-CA	-5.52	115.21	122.99
2	F	345	GLU	N-CA-C	5.52	119.49	112.87
1	G	283	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	283	HIS	CA-CB-CG	-5.51	108.28	113.80
2	D	243	ARG	N-CA-C	5.51	118.47	111.69
2	N	54	ASN	CA-C-N	-5.51	114.86	122.30
2	N	54	ASN	C-N-CA	-5.51	114.86	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	88	ARG	CA-C-N	5.51	125.86	119.47
2	P	88	ARG	C-N-CA	5.51	125.86	119.47
2	H	345	GLU	N-CA-C	5.51	119.48	112.87
1	C	354	GLY	CA-C-N	-5.51	115.51	123.11
1	C	354	GLY	C-N-CA	-5.51	115.51	123.11
2	D	253	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	O	345	ASP	N-CA-C	5.51	122.53	110.80
1	M	309	HIS	CA-C-N	-5.50	116.82	122.27
1	M	309	HIS	C-N-CA	-5.50	116.82	122.27
1	C	319	TYR	N-CA-C	5.50	118.44	109.59
1	G	319	TYR	N-CA-C	5.50	118.44	109.59
1	I	354	GLY	CA-C-N	-5.50	115.52	123.11
1	I	354	GLY	C-N-CA	-5.50	115.52	123.11
1	O	354	GLY	CA-C-N	-5.50	115.52	123.11
1	O	354	GLY	C-N-CA	-5.50	115.52	123.11
1	A	345	ASP	N-CA-C	5.50	122.51	110.80
1	A	354	GLY	CA-C-N	-5.50	115.53	123.11
1	A	354	GLY	C-N-CA	-5.50	115.53	123.11
2	P	54	ASN	CA-C-N	-5.50	114.88	122.30
2	P	54	ASN	C-N-CA	-5.50	114.88	122.30
1	K	345	ASP	N-CA-C	5.50	122.50	110.80
1	C	345	ASP	N-CA-C	5.49	122.50	110.80
1	E	309	HIS	CA-C-N	-5.49	116.83	122.27
1	E	309	HIS	C-N-CA	-5.49	116.83	122.27
2	F	253	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	K	283	HIS	CA-CB-CG	-5.49	108.31	113.80
1	K	354	GLY	CA-C-N	-5.49	115.53	123.11
1	K	354	GLY	C-N-CA	-5.49	115.53	123.11
2	F	54	ASN	CA-C-N	-5.49	114.89	122.30
2	F	54	ASN	C-N-CA	-5.49	114.89	122.30
1	G	345	ASP	N-CA-C	5.49	122.50	110.80
2	J	88	ARG	CA-C-N	5.49	125.84	119.47
2	J	88	ARG	C-N-CA	5.49	125.84	119.47
1	Q	345	ASP	N-CA-C	5.49	122.50	110.80
1	C	283	HIS	CA-CB-CG	-5.49	108.31	113.80
2	J	345	GLU	N-CA-C	5.49	119.46	112.87
1	E	319	TYR	N-CA-C	5.49	118.42	109.59
2	L	88	ARG	CA-C-N	5.49	125.83	119.47
2	L	88	ARG	C-N-CA	5.49	125.83	119.47
1	I	345	ASP	N-CA-C	5.49	122.48	110.80
2	L	345	GLU	N-CA-C	5.49	119.45	112.87
2	N	253	ARG	NE-CZ-NH2	5.49	124.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	HIS	CA-C-N	-5.48	116.84	122.27
1	A	309	HIS	C-N-CA	-5.48	116.84	122.27
1	Q	354	GLY	CA-C-N	-5.48	115.55	123.11
1	Q	354	GLY	C-N-CA	-5.48	115.55	123.11
1	G	309	HIS	CA-C-N	-5.48	116.84	122.27
1	G	309	HIS	C-N-CA	-5.48	116.84	122.27
2	H	54	ASN	CA-C-N	-5.48	114.90	122.30
2	H	54	ASN	C-N-CA	-5.48	114.90	122.30
2	J	253	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	B	253	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	E	354	GLY	CA-C-N	-5.48	115.55	123.11
1	E	354	GLY	C-N-CA	-5.48	115.55	123.11
2	P	345	GLU	N-CA-C	5.48	119.44	112.87
2	B	345	GLU	N-CA-C	5.48	119.44	112.87
2	N	345	GLU	N-CA-C	5.48	119.44	112.87
2	B	54	ASN	CA-C-N	-5.48	114.91	122.30
2	B	54	ASN	C-N-CA	-5.48	114.91	122.30
2	P	253	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	319	TYR	N-CA-C	5.47	118.40	109.59
1	M	354	GLY	CA-C-N	-5.47	115.56	123.11
1	M	354	GLY	C-N-CA	-5.47	115.56	123.11
2	R	88	ARG	CA-C-N	5.47	125.82	119.47
2	R	88	ARG	C-N-CA	5.47	125.82	119.47
2	F	88	ARG	CA-C-N	5.47	125.82	119.47
2	F	88	ARG	C-N-CA	5.47	125.82	119.47
1	M	345	ASP	N-CA-C	5.47	122.46	110.80
2	R	253	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	L	54	ASN	CA-C-N	-5.47	114.91	122.30
2	L	54	ASN	C-N-CA	-5.47	114.91	122.30
1	C	309	HIS	CA-C-N	-5.47	116.85	122.27
1	C	309	HIS	C-N-CA	-5.47	116.85	122.27
1	K	309	HIS	CA-C-N	-5.47	116.86	122.27
1	K	309	HIS	C-N-CA	-5.47	116.86	122.27
1	K	319	TYR	N-CA-C	5.47	118.39	109.59
1	Q	309	HIS	CA-C-N	-5.47	116.86	122.27
1	Q	309	HIS	C-N-CA	-5.47	116.86	122.27
2	B	88	ARG	CA-C-N	5.47	125.81	119.47
2	B	88	ARG	C-N-CA	5.47	125.81	119.47
1	O	309	HIS	CA-C-N	-5.47	116.86	122.27
1	O	309	HIS	C-N-CA	-5.47	116.86	122.27
2	R	345	GLU	N-CA-C	5.47	119.43	112.87
2	D	345	GLU	N-CA-C	5.46	119.42	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	253	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	M	319	TYR	N-CA-C	5.46	118.38	109.59
1	O	319	TYR	N-CA-C	5.46	118.38	109.59
2	D	54	ASN	CA-C-N	-5.46	114.93	122.30
2	D	54	ASN	C-N-CA	-5.46	114.93	122.30
2	R	54	ASN	CA-C-N	-5.46	114.93	122.30
2	R	54	ASN	C-N-CA	-5.46	114.93	122.30
2	N	88	ARG	CA-C-N	5.46	125.80	119.47
2	N	88	ARG	C-N-CA	5.46	125.80	119.47
1	I	319	TYR	N-CA-C	5.45	118.37	109.59
2	L	253	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Q	319	TYR	N-CA-C	5.45	118.37	109.59
2	H	88	ARG	CA-C-N	5.45	125.79	119.47
2	H	88	ARG	C-N-CA	5.45	125.79	119.47
2	D	88	ARG	CA-C-N	5.44	125.78	119.47
2	D	88	ARG	C-N-CA	5.44	125.78	119.47
2	J	54	ASN	CA-C-N	-5.44	114.95	122.30
2	J	54	ASN	C-N-CA	-5.44	114.95	122.30
1	E	101	ASN	CA-C-N	-5.44	113.55	121.76
1	E	101	ASN	C-N-CA	-5.44	113.55	121.76
1	I	101	ASN	CA-C-N	-5.44	113.55	121.76
1	I	101	ASN	C-N-CA	-5.44	113.55	121.76
1	O	101	ASN	CA-C-N	-5.43	113.55	121.76
1	O	101	ASN	C-N-CA	-5.43	113.55	121.76
1	G	101	ASN	CA-C-N	-5.43	113.56	121.76
1	G	101	ASN	C-N-CA	-5.43	113.56	121.76
1	Q	101	ASN	CA-C-N	-5.43	113.57	121.76
1	Q	101	ASN	C-N-CA	-5.43	113.57	121.76
1	C	101	ASN	CA-C-N	-5.42	113.57	121.76
1	C	101	ASN	C-N-CA	-5.42	113.57	121.76
2	H	308	ARG	CD-NE-CZ	5.42	131.99	124.40
1	M	101	ASN	CA-C-N	-5.42	113.58	121.76
1	M	101	ASN	C-N-CA	-5.42	113.58	121.76
2	H	277	SER	CA-C-N	5.41	128.28	120.38
2	H	277	SER	C-N-CA	5.41	128.28	120.38
2	B	356	CYS	CA-C-N	-5.41	113.61	122.54
2	B	356	CYS	C-N-CA	-5.41	113.61	122.54
2	J	356	CYS	CA-C-N	-5.41	113.61	122.54
2	J	356	CYS	C-N-CA	-5.41	113.61	122.54
2	N	308	ARG	CD-NE-CZ	5.41	131.98	124.40
2	N	356	CYS	CA-C-N	-5.41	113.61	122.54
2	N	356	CYS	C-N-CA	-5.41	113.61	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASN	CA-C-N	-5.41	113.59	121.76
1	A	101	ASN	C-N-CA	-5.41	113.59	121.76
2	R	308	ARG	CD-NE-CZ	5.41	131.97	124.40
2	D	81	GLY	CA-C-N	5.40	125.33	119.76
2	D	81	GLY	C-N-CA	5.40	125.33	119.76
2	F	356	CYS	CA-C-N	-5.40	113.63	122.54
2	F	356	CYS	C-N-CA	-5.40	113.63	122.54
2	J	81	GLY	CA-C-N	5.40	125.32	119.76
2	J	81	GLY	C-N-CA	5.40	125.32	119.76
2	J	277	SER	CA-C-N	5.40	128.27	120.38
2	J	277	SER	C-N-CA	5.40	128.27	120.38
2	L	356	CYS	CA-C-N	-5.40	113.63	122.54
2	L	356	CYS	C-N-CA	-5.40	113.63	122.54
2	D	356	CYS	CA-C-N	-5.40	113.63	122.54
2	D	356	CYS	C-N-CA	-5.40	113.63	122.54
2	P	356	CYS	CA-C-N	-5.40	113.63	122.54
2	P	356	CYS	C-N-CA	-5.40	113.63	122.54
2	R	81	GLY	CA-C-N	5.40	125.32	119.76
2	R	81	GLY	C-N-CA	5.40	125.32	119.76
2	D	277	SER	CA-C-N	5.40	128.26	120.38
2	D	277	SER	C-N-CA	5.40	128.26	120.38
2	F	277	SER	CA-C-N	5.40	128.26	120.38
2	F	277	SER	C-N-CA	5.40	128.26	120.38
2	H	356	CYS	CA-C-N	-5.40	113.63	122.54
2	H	356	CYS	C-N-CA	-5.40	113.63	122.54
2	L	308	ARG	CD-NE-CZ	5.40	131.95	124.40
1	K	101	ASN	CA-C-N	-5.39	113.61	121.76
1	K	101	ASN	C-N-CA	-5.39	113.61	121.76
2	P	81	GLY	CA-C-N	5.39	125.32	119.76
2	P	81	GLY	C-N-CA	5.39	125.32	119.76
2	B	277	SER	CA-C-N	5.39	128.25	120.38
2	B	277	SER	C-N-CA	5.39	128.25	120.38
2	R	356	CYS	CA-C-N	-5.39	113.64	122.54
2	R	356	CYS	C-N-CA	-5.39	113.64	122.54
2	B	308	ARG	CD-NE-CZ	5.39	131.95	124.40
2	L	277	SER	CA-C-N	5.39	128.25	120.38
2	L	277	SER	C-N-CA	5.39	128.25	120.38
2	D	308	ARG	CD-NE-CZ	5.39	131.94	124.40
2	H	81	GLY	CA-C-N	5.39	125.31	119.76
2	H	81	GLY	C-N-CA	5.39	125.31	119.76
2	B	81	GLY	CA-C-N	5.38	125.30	119.76
2	B	81	GLY	C-N-CA	5.38	125.30	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	81	GLY	CA-C-N	5.38	125.30	119.76
2	N	81	GLY	C-N-CA	5.38	125.30	119.76
2	J	272	PHE	N-CA-C	5.38	117.94	108.75
2	L	81	GLY	CA-C-N	5.38	125.30	119.76
2	L	81	GLY	C-N-CA	5.38	125.30	119.76
2	P	272	PHE	N-CA-C	5.38	117.94	108.75
2	F	81	GLY	CA-C-N	5.37	125.29	119.76
2	F	81	GLY	C-N-CA	5.37	125.29	119.76
2	F	308	ARG	CD-NE-CZ	5.37	131.92	124.40
2	R	277	SER	CA-C-N	5.37	128.22	120.38
2	R	277	SER	C-N-CA	5.37	128.22	120.38
2	B	272	PHE	N-CA-C	5.37	117.93	108.75
2	N	277	SER	CA-C-N	5.37	128.22	120.38
2	N	277	SER	C-N-CA	5.37	128.22	120.38
2	D	272	PHE	N-CA-C	5.37	117.92	108.75
2	R	272	PHE	N-CA-C	5.36	117.92	108.75
2	J	264	ARG	N-CA-C	5.36	119.97	113.38
2	D	264	ARG	N-CA-C	5.36	119.97	113.38
2	H	296	PHE	CA-CB-CG	-5.36	108.44	113.80
2	L	272	PHE	N-CA-C	5.36	117.91	108.75
2	P	308	ARG	CD-NE-CZ	5.36	131.90	124.40
2	N	272	PHE	N-CA-C	5.36	117.91	108.75
2	P	277	SER	CA-C-N	5.35	128.20	120.38
2	P	277	SER	C-N-CA	5.35	128.20	120.38
1	E	123	ARG	NE-CZ-NH2	-5.35	114.38	119.20
2	J	308	ARG	CD-NE-CZ	5.35	131.89	124.40
2	F	272	PHE	N-CA-C	5.35	117.90	108.75
1	O	123	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	A	123	ARG	NE-CZ-NH2	-5.35	114.39	119.20
2	B	264	ARG	N-CA-C	5.35	119.95	113.38
1	Q	123	ARG	NE-CZ-NH2	-5.35	114.39	119.20
2	L	264	ARG	N-CA-C	5.34	119.95	113.38
2	F	264	ARG	N-CA-C	5.34	119.95	113.38
2	N	185	TYR	CA-CB-CG	5.34	123.52	113.90
2	P	264	ARG	N-CA-C	5.34	119.95	113.38
1	I	156	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	D	296	PHE	CA-CB-CG	-5.34	108.46	113.80
2	H	272	PHE	N-CA-C	5.34	117.88	108.75
2	D	185	TYR	CA-CB-CG	5.34	123.50	113.90
1	O	109	THR	N-CA-C	5.33	122.16	110.80
2	R	264	ARG	N-CA-C	5.33	119.94	113.38
2	B	185	TYR	CA-CB-CG	5.33	123.50	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	185	TYR	CA-CB-CG	5.33	123.50	113.90
1	C	123	ARG	NE-CZ-NH2	-5.33	114.41	119.20
2	N	264	ARG	N-CA-C	5.33	119.93	113.38
1	G	55	GLU	N-CA-C	5.33	118.91	109.96
2	H	264	ARG	N-CA-C	5.33	119.93	113.38
1	K	123	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	O	205	ASP	CA-CB-CG	5.33	117.93	112.60
2	P	185	TYR	CA-CB-CG	5.33	123.48	113.90
2	P	296	PHE	CA-CB-CG	-5.33	108.47	113.80
1	O	245	ASP	N-CA-C	5.32	118.16	110.28
2	H	185	TYR	CA-CB-CG	5.32	123.48	113.90
1	Q	135	PHE	N-CA-C	5.32	116.37	108.60
2	B	296	PHE	CA-CB-CG	-5.32	108.48	113.80
2	L	296	PHE	CA-CB-CG	-5.32	108.48	113.80
1	C	55	GLU	N-CA-C	5.32	118.89	109.96
1	M	109	THR	N-CA-C	5.32	122.12	110.80
2	R	185	TYR	CA-CB-CG	5.32	123.47	113.90
2	F	185	TYR	CA-CB-CG	5.32	123.47	113.90
2	F	296	PHE	CA-CB-CG	-5.32	108.48	113.80
1	I	123	ARG	NE-CZ-NH2	-5.32	114.42	119.20
1	C	109	THR	N-CA-C	5.31	122.12	110.80
2	N	296	PHE	CA-CB-CG	-5.31	108.49	113.80
1	E	205	ASP	CA-CB-CG	5.31	117.91	112.60
1	M	123	ARG	NE-CZ-NH2	-5.31	114.42	119.20
2	J	296	PHE	CA-CB-CG	-5.31	108.49	113.80
1	Q	109	THR	N-CA-C	5.31	122.11	110.80
1	A	55	GLU	N-CA-C	5.31	118.88	109.96
1	A	205	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	109	THR	N-CA-C	5.31	122.11	110.80
2	R	405	LEU	N-CA-CB	5.31	119.33	110.41
1	K	55	GLU	N-CA-C	5.31	118.87	109.96
2	L	185	TYR	CA-CB-CG	5.31	123.45	113.90
1	I	109	THR	N-CA-C	5.30	122.10	110.80
1	M	55	GLU	N-CA-C	5.30	118.87	109.96
1	Q	205	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	109	THR	N-CA-C	5.30	122.09	110.80
1	E	55	GLU	N-CA-C	5.30	118.87	109.96
1	G	123	ARG	NE-CZ-NH2	-5.30	114.43	119.20
2	B	405	LEU	N-CA-CB	5.30	119.31	110.41
2	P	405	LEU	N-CA-CB	5.30	119.31	110.41
2	R	296	PHE	CA-CB-CG	-5.30	108.50	113.80
1	E	109	THR	N-CA-C	5.30	122.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	405	LEU	N-CA-CB	5.30	119.31	110.41
1	I	55	GLU	N-CA-C	5.30	118.86	109.96
1	K	109	THR	N-CA-C	5.30	122.08	110.80
1	E	135	PHE	N-CA-C	5.30	116.33	108.60
2	L	212	ILE	CB-CA-C	-5.30	104.99	112.14
1	K	245	ASP	N-CA-C	5.29	118.12	110.28
1	M	205	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	135	PHE	N-CA-C	5.29	116.33	108.60
1	A	156	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	C	156	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	L	405	LEU	N-CA-CB	5.29	119.30	110.41
2	N	96	GLN	O-C-N	5.29	129.45	122.36
1	Q	55	GLU	N-CA-C	5.29	118.85	109.96
1	G	245	ASP	N-CA-C	5.29	118.11	110.28
1	O	55	GLU	N-CA-C	5.29	118.85	109.96
1	M	156	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	D	405	LEU	N-CA-CB	5.29	119.29	110.41
1	G	135	PHE	N-CA-C	5.29	116.32	108.60
1	O	135	PHE	N-CA-C	5.29	116.32	108.60
1	C	135	PHE	N-CA-C	5.29	116.32	108.60
2	J	405	LEU	N-CA-CB	5.29	119.29	110.41
2	N	405	LEU	N-CA-CB	5.29	119.29	110.41
1	E	245	ASP	N-CA-C	5.28	118.10	110.28
1	M	245	ASP	N-CA-C	5.28	118.10	110.28
1	I	135	PHE	N-CA-C	5.28	116.31	108.60
1	K	135	PHE	N-CA-C	5.28	116.31	108.60
1	E	379	SER	N-CA-C	5.28	117.78	108.75
2	R	228	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	245	ASP	N-CA-C	5.28	118.09	110.28
1	G	156	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	H	212	ILE	CB-CA-C	-5.28	105.02	112.14
2	H	405	LEU	N-CA-CB	5.28	119.27	110.41
2	L	166	MET	CA-C-N	-5.28	113.96	122.82
2	L	166	MET	C-N-CA	-5.28	113.96	122.82
1	M	135	PHE	N-CA-C	5.28	116.30	108.60
1	Q	156	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	K	205	ASP	CA-CB-CG	5.27	117.87	112.60
1	I	205	ASP	CA-CB-CG	5.27	117.87	112.60
2	P	350	ASN	N-CA-C	5.27	122.03	110.80
2	F	350	ASN	N-CA-C	5.27	122.02	110.80
1	M	379	SER	N-CA-C	5.27	117.76	108.75
1	Q	245	ASP	N-CA-C	5.27	118.08	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ASP	CA-CB-CG	5.27	117.87	112.60
2	D	212	ILE	CB-CA-C	-5.27	105.03	112.14
2	J	350	ASN	N-CA-C	5.27	122.02	110.80
2	B	212	ILE	CB-CA-C	-5.26	105.03	112.14
2	D	203	CYS	N-CA-C	5.26	117.54	107.75
2	F	203	CYS	N-CA-C	5.26	117.54	107.75
1	K	156	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	P	212	ILE	CB-CA-C	-5.26	105.03	112.14
1	C	379	SER	N-CA-C	5.26	117.75	108.75
2	D	166	MET	CA-C-N	-5.26	113.98	122.82
2	D	166	MET	C-N-CA	-5.26	113.98	122.82
1	G	205	ASP	CA-CB-CG	5.26	117.86	112.60
2	J	166	MET	CA-C-N	-5.26	113.98	122.82
2	J	166	MET	C-N-CA	-5.26	113.98	122.82
2	N	212	ILE	CB-CA-C	-5.26	105.04	112.14
1	O	379	SER	N-CA-C	5.26	117.75	108.75
2	B	350	ASN	N-CA-C	5.26	122.00	110.80
1	C	245	ASP	N-CA-C	5.26	118.06	110.28
1	I	379	SER	N-CA-C	5.26	117.74	108.75
2	J	212	ILE	CB-CA-C	-5.26	105.04	112.14
1	O	156	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	G	259	LEU	N-CA-C	5.26	120.70	113.97
1	G	379	SER	N-CA-C	5.26	117.74	108.75
2	J	203	CYS	N-CA-C	5.26	117.53	107.75
2	L	350	ASN	N-CA-C	5.26	122.00	110.80
2	N	203	CYS	N-CA-C	5.26	117.53	107.75
2	R	212	ILE	CB-CA-C	-5.26	105.04	112.14
1	A	379	SER	N-CA-C	5.26	117.74	108.75
2	B	166	MET	CA-C-N	-5.26	113.99	122.82
2	B	166	MET	C-N-CA	-5.26	113.99	122.82
2	F	166	MET	CA-C-N	-5.26	113.99	122.82
2	F	166	MET	C-N-CA	-5.26	113.99	122.82
1	K	379	SER	N-CA-C	5.26	117.74	108.75
2	L	203	CYS	N-CA-C	5.26	117.53	107.75
2	N	350	ASN	N-CA-C	5.26	122.00	110.80
2	R	350	ASN	N-CA-C	5.26	122.00	110.80
2	F	212	ILE	CB-CA-C	-5.25	105.05	112.14
2	P	166	MET	CA-C-N	-5.25	113.99	122.82
2	P	166	MET	C-N-CA	-5.25	113.99	122.82
2	F	96	GLN	O-C-N	5.25	129.40	122.36
1	Q	264	ARG	O-C-N	5.25	128.83	122.68
2	B	203	CYS	N-CA-C	5.25	117.52	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	259	LEU	N-CA-C	5.25	120.69	113.97
2	N	166	MET	CA-C-N	-5.25	114.00	122.82
2	N	166	MET	C-N-CA	-5.25	114.00	122.82
2	P	203	CYS	N-CA-C	5.25	117.52	107.75
2	P	228	ASN	CA-CB-CG	-5.25	107.35	112.60
2	D	228	ASN	CA-CB-CG	-5.25	107.35	112.60
1	E	334	THR	CA-C-N	-5.25	111.92	120.64
1	E	334	THR	C-N-CA	-5.25	111.92	120.64
1	Q	379	SER	N-CA-C	5.25	117.73	108.75
2	D	350	ASN	N-CA-C	5.25	121.98	110.80
1	E	156	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	F	122	VAL	CB-CA-C	-5.25	105.25	111.97
2	H	166	MET	CA-C-N	-5.25	114.00	122.82
2	H	166	MET	C-N-CA	-5.25	114.00	122.82
1	I	245	ASP	N-CA-C	5.25	118.05	110.28
2	L	228	ASN	CA-CB-CG	-5.25	107.35	112.60
2	R	203	CYS	N-CA-C	5.25	117.51	107.75
2	B	228	ASN	CA-CB-CG	-5.25	107.36	112.60
1	A	259	LEU	N-CA-C	5.24	120.68	113.97
1	Q	259	LEU	N-CA-C	5.24	120.68	113.97
2	H	203	CYS	N-CA-C	5.24	117.49	107.75
2	H	350	ASN	N-CA-C	5.24	121.96	110.80
1	C	264	ARG	O-C-N	5.24	128.81	122.68
2	N	228	ASN	CA-CB-CG	-5.24	107.36	112.60
1	C	334	THR	CA-C-N	-5.24	111.95	120.64
1	C	334	THR	C-N-CA	-5.24	111.95	120.64
2	J	228	ASN	CA-CB-CG	-5.24	107.36	112.60
1	C	259	LEU	N-CA-C	5.23	120.67	113.97
1	M	259	LEU	N-CA-C	5.23	120.67	113.97
2	N	122	VAL	CB-CA-C	-5.23	105.27	111.97
1	O	334	THR	CA-C-N	-5.23	111.95	120.64
1	O	334	THR	C-N-CA	-5.23	111.95	120.64
1	O	259	LEU	N-CA-C	5.23	120.67	113.97
2	R	166	MET	CA-C-N	-5.23	114.03	122.82
2	R	166	MET	C-N-CA	-5.23	114.03	122.82
2	D	122	VAL	CB-CA-C	-5.23	105.28	111.97
2	B	122	VAL	CB-CA-C	-5.22	105.28	111.97
2	F	228	ASN	CA-CB-CG	-5.22	107.38	112.60
1	G	264	ARG	O-C-N	5.22	128.79	122.68
1	I	334	THR	CA-C-N	-5.22	111.97	120.64
1	I	334	THR	C-N-CA	-5.22	111.97	120.64
1	M	334	THR	CA-C-N	-5.22	111.97	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	334	THR	C-N-CA	-5.22	111.97	120.64
1	K	259	LEU	N-CA-C	5.22	120.66	113.97
2	P	122	VAL	CB-CA-C	-5.22	105.29	111.97
2	H	228	ASN	CA-CB-CG	-5.22	107.38	112.60
1	K	264	ARG	O-C-N	5.22	128.79	122.68
1	A	334	THR	CA-C-N	-5.22	111.98	120.64
1	A	334	THR	C-N-CA	-5.22	111.98	120.64
1	E	259	LEU	N-CA-C	5.22	120.65	113.97
1	E	264	ARG	O-C-N	5.21	128.78	122.68
2	H	122	VAL	CB-CA-C	-5.21	105.30	111.97
2	J	122	VAL	CB-CA-C	-5.20	105.31	111.97
1	O	264	ARG	O-C-N	5.20	128.77	122.68
2	P	238	VAL	CA-C-N	-5.20	112.50	121.66
2	P	238	VAL	C-N-CA	-5.20	112.50	121.66
1	Q	334	THR	CA-C-N	-5.20	112.01	120.64
1	Q	334	THR	C-N-CA	-5.20	112.01	120.64
2	R	122	VAL	CB-CA-C	-5.20	105.31	111.97
1	A	264	ARG	O-C-N	5.19	128.76	122.68
1	G	334	THR	CA-C-N	-5.19	112.02	120.64
1	G	334	THR	C-N-CA	-5.19	112.02	120.64
1	K	334	THR	CA-C-N	-5.19	112.02	120.64
1	K	334	THR	C-N-CA	-5.19	112.02	120.64
2	L	238	VAL	CA-C-N	-5.19	112.52	121.66
2	L	238	VAL	C-N-CA	-5.19	112.52	121.66
2	N	238	VAL	CA-C-N	-5.19	112.52	121.66
2	N	238	VAL	C-N-CA	-5.19	112.52	121.66
2	D	238	VAL	CA-C-N	-5.19	112.53	121.66
2	D	238	VAL	C-N-CA	-5.19	112.53	121.66
2	B	238	VAL	CA-C-N	-5.19	112.53	121.66
2	B	238	VAL	C-N-CA	-5.19	112.53	121.66
1	M	264	ARG	O-C-N	5.19	128.75	122.68
2	P	226	ASP	N-CA-C	-5.18	106.11	112.90
2	R	238	VAL	CA-C-N	-5.18	112.54	121.66
2	R	238	VAL	C-N-CA	-5.18	112.54	121.66
2	L	122	VAL	CB-CA-C	-5.18	105.34	111.97
2	D	226	ASP	N-CA-C	-5.17	106.13	112.90
2	H	238	VAL	CA-C-N	-5.17	112.56	121.66
2	H	238	VAL	C-N-CA	-5.17	112.56	121.66
2	J	238	VAL	CA-C-N	-5.17	112.56	121.66
2	J	238	VAL	C-N-CA	-5.17	112.56	121.66
1	K	98	ASP	O-C-N	5.17	128.73	122.94
2	F	238	VAL	CA-C-N	-5.17	112.56	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	238	VAL	C-N-CA	-5.17	112.56	121.66
1	C	138	PHE	CA-CB-CG	-5.17	108.63	113.80
1	O	138	PHE	CA-CB-CG	-5.17	108.63	113.80
1	Q	138	PHE	CA-CB-CG	-5.17	108.63	113.80
2	J	47	GLU	N-CA-C	5.16	119.89	111.37
2	F	226	ASP	N-CA-C	-5.16	106.14	112.90
2	L	226	ASP	N-CA-C	-5.16	106.14	112.90
1	M	98	ASP	O-C-N	5.16	128.72	122.94
2	B	226	ASP	N-CA-C	-5.16	106.15	112.90
2	F	47	GLU	N-CA-C	5.16	119.88	111.37
1	M	138	PHE	CA-CB-CG	-5.16	108.64	113.80
2	J	226	ASP	N-CA-C	-5.15	106.15	112.90
2	R	47	GLU	N-CA-C	5.15	119.87	111.37
1	A	138	PHE	CA-CB-CG	-5.15	108.65	113.80
1	K	138	PHE	CA-CB-CG	-5.15	108.65	113.80
1	I	264	ARG	O-C-N	5.15	128.70	122.68
2	N	226	ASP	N-CA-C	-5.15	106.16	112.90
1	G	138	PHE	CA-CB-CG	-5.14	108.66	113.80
2	H	47	GLU	N-CA-C	5.14	119.86	111.37
2	N	47	GLU	N-CA-C	5.14	119.86	111.37
2	B	47	GLU	N-CA-C	5.14	119.85	111.37
1	G	98	ASP	O-C-N	5.14	128.70	122.94
2	H	226	ASP	N-CA-C	-5.14	106.17	112.90
1	O	98	ASP	O-C-N	5.14	128.70	122.94
2	D	47	GLU	N-CA-C	5.14	119.85	111.37
1	I	138	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	98	ASP	O-C-N	5.13	128.68	122.94
2	R	226	ASP	N-CA-C	-5.13	106.18	112.90
2	P	47	GLU	N-CA-C	5.12	119.82	111.37
1	Q	98	ASP	O-C-N	5.12	128.67	122.94
1	I	98	ASP	O-C-N	5.12	128.67	122.94
2	L	47	GLU	N-CA-C	5.12	119.81	111.37
1	E	138	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	98	ASP	O-C-N	5.11	128.66	122.94
1	G	339	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
1	E	98	ASP	O-C-N	5.09	128.64	122.94
1	O	339	ARG	NH1-CZ-NH2	-5.08	112.70	119.30
1	Q	300	ASN	CA-CB-CG	-5.07	107.53	112.60
1	E	300	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	339	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
1	E	339	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
2	R	139	HIS	CA-CB-CG	-5.06	108.74	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	339	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	I	339	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
2	J	139	HIS	CA-CB-CG	-5.06	108.74	113.80
1	K	339	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
2	P	139	HIS	CA-CB-CG	-5.05	108.75	113.80
2	N	139	HIS	CA-CB-CG	-5.05	108.75	113.80
1	Q	339	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	M	121	ARG	NE-CZ-NH1	-5.05	116.45	121.50
2	N	97	SER	O-C-N	5.05	129.60	123.14
2	D	139	HIS	CA-CB-CG	-5.05	108.75	113.80
2	F	400	ARG	NE-CZ-NH1	-5.05	116.45	121.50
2	H	139	HIS	CA-CB-CG	-5.05	108.75	113.80
1	M	300	ASN	CA-CB-CG	-5.05	107.55	112.60
2	B	139	HIS	CA-CB-CG	-5.04	108.75	113.80
2	H	97	SER	O-C-N	5.04	129.59	123.14
2	R	97	SER	O-C-N	5.04	129.59	123.14
1	I	300	ASN	CA-CB-CG	-5.04	107.56	112.60
2	J	400	ARG	NE-CZ-NH1	-5.04	116.47	121.50
2	F	139	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	300	ASN	CA-CB-CG	-5.03	107.57	112.60
2	L	400	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	I	121	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	M	339	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
2	B	97	SER	O-C-N	5.02	129.57	123.14
2	L	139	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	121	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	D	97	SER	O-C-N	5.02	129.57	123.14
1	K	300	ASN	CA-CB-CG	-5.02	107.58	112.60
2	H	400	ARG	NE-CZ-NH1	-5.02	116.48	121.50
2	N	400	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	I	214	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	O	121	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	P	97	SER	O-C-N	5.01	129.56	123.14
1	G	300	ASN	CA-CB-CG	-5.01	107.59	112.60
2	H	356	CYS	N-CA-CB	-5.01	102.11	110.83
2	J	356	CYS	N-CA-CB	-5.01	102.11	110.83
2	D	260	VAL	CA-C-N	5.01	124.70	119.64
2	D	260	VAL	C-N-CA	5.01	124.70	119.64
2	J	260	VAL	CA-C-N	5.01	124.70	119.64
2	J	260	VAL	C-N-CA	5.01	124.70	119.64
2	D	356	CYS	N-CA-CB	-5.01	102.12	110.83
2	P	400	ARG	NE-CZ-NH1	-5.01	116.49	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	C	300	ASN	CA-CB-CG	-5.01	107.59	112.60
2	J	97	SER	O-C-N	5.01	129.55	123.14
2	F	260	VAL	CA-C-N	5.00	124.69	119.64
2	F	260	VAL	C-N-CA	5.00	124.69	119.64

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LEU	Peptide
2	D	248	LEU	Peptide
2	F	248	LEU	Peptide
2	H	248	LEU	Peptide
2	J	248	LEU	Peptide
2	L	248	LEU	Peptide
2	N	248	LEU	Peptide
2	P	248	LEU	Peptide
2	R	248	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	39	0
1	C	3350	0	3254	43	0
1	E	3350	0	3254	42	0
1	G	3350	0	3254	42	0
1	I	3350	0	3254	38	0
1	K	3350	0	3254	38	0
1	M	3350	0	3254	41	0
1	O	3350	0	3254	38	0
1	Q	3350	0	3254	40	0
2	B	3352	0	3227	35	0
2	D	3352	0	3227	37	0
2	F	3352	0	3227	37	0
2	H	3352	0	3227	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	3352	0	3227	33	0
2	L	3352	0	3227	38	0
2	N	3352	0	3227	40	0
2	P	3352	0	3227	45	0
2	R	3352	0	3227	43	0
3	A	32	0	12	2	0
3	C	32	0	12	2	0
3	E	32	0	12	2	0
3	G	32	0	12	2	0
3	I	32	0	12	2	0
3	K	32	0	12	2	0
3	M	32	0	12	2	0
3	O	32	0	12	2	0
3	Q	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0
5	P	28	0	12	2	0
5	R	28	0	12	2	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
6	E	4	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	K	4	0	0	0	0
6	M	4	0	0	0	0
6	O	4	0	0	0	0
6	Q	4	0	0	0	0
All	All	60903	0	58545	664	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (664) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:228:ASN:HD21	5:J:901:GDP:HN1	1.17	0.91
2:L:228:ASN:HD21	5:L:901:GDP:HN1	1.17	0.90
2:B:228:ASN:HD21	5:B:901:GDP:HN1	1.17	0.90
2:F:228:ASN:HD21	5:F:901:GDP:HN1	1.17	0.90
2:R:228:ASN:HD21	5:R:901:GDP:HN1	1.17	0.90
2:P:228:ASN:HD21	5:P:901:GDP:HN1	1.17	0.90
2:H:228:ASN:HD21	5:H:901:GDP:HN1	1.17	0.88
2:D:228:ASN:HD21	5:D:901:GDP:HN1	1.17	0.88
2:N:228:ASN:HD21	5:N:901:GDP:HN1	1.17	0.87
1:K:238:ILE:O	1:K:238:ILE:HG22	1.77	0.84
1:E:238:ILE:HG22	1:E:238:ILE:O	1.78	0.83
1:G:238:ILE:HG22	1:G:238:ILE:O	1.78	0.83
1:Q:238:ILE:HG22	1:Q:238:ILE:O	1.77	0.83
1:C:238:ILE:HG22	1:C:238:ILE:O	1.78	0.83
1:M:238:ILE:HG22	1:M:238:ILE:O	1.77	0.83
1:I:238:ILE:O	1:I:238:ILE:HG22	1.77	0.82
1:A:238:ILE:O	1:A:238:ILE:HG22	1.77	0.81
1:O:238:ILE:HG22	1:O:238:ILE:O	1.77	0.81
2:L:345:GLU:OE1	2:L:345:GLU:N	2.16	0.79
2:H:345:GLU:OE1	2:H:345:GLU:N	2.16	0.78
2:J:345:GLU:OE1	2:J:345:GLU:N	2.16	0.76
2:B:345:GLU:OE1	2:B:345:GLU:N	2.16	0.76
2:P:345:GLU:OE1	2:P:345:GLU:N	2.16	0.76
2:F:345:GLU:OE1	2:F:345:GLU:N	2.16	0.73
2:N:345:GLU:OE1	2:N:345:GLU:N	2.16	0.73
2:R:345:GLU:OE1	2:R:345:GLU:N	2.16	0.73
2:D:345:GLU:OE1	2:D:345:GLU:N	2.16	0.73
2:F:266:HIS:O	2:F:266:HIS:ND1	2.22	0.72
2:L:266:HIS:O	2:L:266:HIS:ND1	2.22	0.72
2:R:266:HIS:O	2:R:266:HIS:ND1	2.22	0.72
2:D:266:HIS:O	2:D:266:HIS:ND1	2.22	0.71
2:H:266:HIS:O	2:H:266:HIS:ND1	2.22	0.71
2:P:266:HIS:ND1	2:P:266:HIS:O	2.22	0.71
2:B:266:HIS:O	2:B:266:HIS:ND1	2.22	0.71
2:J:266:HIS:O	2:J:266:HIS:ND1	2.22	0.71
2:N:266:HIS:O	2:N:266:HIS:ND1	2.22	0.70
1:Q:238:ILE:O	1:Q:238:ILE:CG2	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:O	1:E:238:ILE:CG2	2.40	0.70
1:K:238:ILE:O	1:K:238:ILE:CG2	2.40	0.70
1:O:238:ILE:O	1:O:238:ILE:CG2	2.40	0.69
1:C:238:ILE:O	1:C:238:ILE:CG2	2.40	0.69
1:G:238:ILE:O	1:G:238:ILE:CG2	2.40	0.69
1:A:238:ILE:O	1:A:238:ILE:CG2	2.40	0.69
1:M:238:ILE:O	1:M:238:ILE:CG2	2.40	0.69
2:D:332:MET:HE2	2:D:332:MET:HA	1.75	0.69
2:H:332:MET:HE2	2:H:332:MET:HA	1.75	0.69
2:N:332:MET:HA	2:N:332:MET:HE2	1.75	0.69
2:F:332:MET:HE2	2:F:332:MET:HA	1.75	0.69
2:L:332:MET:HA	2:L:332:MET:HE2	1.75	0.69
2:R:332:MET:HE2	2:R:332:MET:HA	1.75	0.69
2:P:284:ARG:NH1	2:R:90:ASP:OD2	2.27	0.68
2:P:332:MET:HE2	2:P:332:MET:HA	1.75	0.68
2:B:332:MET:HA	2:B:332:MET:HE2	1.75	0.68
2:J:332:MET:HE2	2:J:332:MET:HA	1.75	0.67
1:I:238:ILE:O	1:I:238:ILE:CG2	2.40	0.67
1:O:243:ARG:HA	1:O:243:ARG:NE	2.10	0.67
1:A:243:ARG:HA	1:A:243:ARG:NE	2.10	0.67
1:G:243:ARG:HA	1:G:243:ARG:NE	2.10	0.66
1:I:243:ARG:HA	1:I:243:ARG:NE	2.10	0.66
1:C:243:ARG:NE	1:C:243:ARG:HA	2.10	0.66
1:M:243:ARG:NE	1:M:243:ARG:HA	2.10	0.66
2:J:381:SER:OG	2:J:382:THR:N	2.29	0.65
1:Q:243:ARG:HA	1:Q:243:ARG:NE	2.10	0.65
1:K:243:ARG:HA	1:K:243:ARG:NE	2.10	0.65
1:E:243:ARG:HA	1:E:243:ARG:NE	2.10	0.65
2:H:381:SER:OG	2:H:382:THR:N	2.29	0.64
1:E:15:GLN:OE1	1:E:15:GLN:HA	1.98	0.64
2:D:381:SER:OG	2:D:382:THR:N	2.29	0.64
1:K:15:GLN:HA	1:K:15:GLN:OE1	1.98	0.64
2:N:381:SER:OG	2:N:382:THR:N	2.29	0.64
1:Q:15:GLN:OE1	1:Q:15:GLN:HA	1.98	0.64
1:A:15:GLN:HA	1:A:15:GLN:OE1	1.98	0.64
1:I:15:GLN:HA	1:I:15:GLN:OE1	1.98	0.64
1:O:15:GLN:OE1	1:O:15:GLN:HA	1.98	0.64
1:G:15:GLN:OE1	1:G:15:GLN:HA	1.98	0.63
1:C:15:GLN:OE1	1:C:15:GLN:HA	1.98	0.63
1:M:15:GLN:HA	1:M:15:GLN:OE1	1.98	0.63
2:D:306:ASP:OD1	2:D:306:ASP:C	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:306:ASP:OD1	2:P:306:ASP:C	2.40	0.62
2:B:306:ASP:OD1	2:B:306:ASP:C	2.40	0.62
2:H:306:ASP:C	2:H:306:ASP:OD1	2.40	0.62
2:J:306:ASP:C	2:J:306:ASP:OD1	2.40	0.62
2:N:306:ASP:OD1	2:N:306:ASP:C	2.40	0.62
2:R:381:SER:OG	2:R:382:THR:N	2.29	0.62
2:F:381:SER:OG	2:F:382:THR:N	2.29	0.62
2:L:381:SER:OG	2:L:382:THR:N	2.29	0.62
1:C:11:GLN:HG2	1:C:74:VAL:HG21	1.84	0.60
1:G:11:GLN:HG2	1:G:74:VAL:HG21	1.84	0.59
2:F:221:THR:N	2:F:222:PRO:HD3	2.17	0.59
2:L:221:THR:N	2:L:222:PRO:HD3	2.17	0.59
1:M:11:GLN:HG2	1:M:74:VAL:HG21	1.84	0.59
1:O:11:GLN:HG2	1:O:74:VAL:HG21	1.84	0.59
1:Q:11:GLN:HG2	1:Q:74:VAL:HG21	1.84	0.59
2:R:221:THR:N	2:R:222:PRO:HD3	2.17	0.59
1:A:11:GLN:HG2	1:A:74:VAL:HG21	1.84	0.59
2:N:284:ARG:NH1	2:P:90:ASP:OD2	2.32	0.59
2:B:221:THR:N	2:B:222:PRO:HD3	2.17	0.59
2:D:221:THR:N	2:D:222:PRO:HD3	2.17	0.59
2:H:221:THR:N	2:H:222:PRO:HD3	2.17	0.59
1:I:11:GLN:HG2	1:I:74:VAL:HG21	1.84	0.59
2:B:381:SER:OG	2:B:382:THR:N	2.29	0.59
2:N:221:THR:N	2:N:222:PRO:HD3	2.17	0.59
2:P:221:THR:N	2:P:222:PRO:HD3	2.17	0.59
2:R:306:ASP:C	2:R:306:ASP:OD1	2.40	0.59
1:E:11:GLN:HG2	1:E:74:VAL:HG21	1.84	0.59
2:J:221:THR:N	2:J:222:PRO:HD3	2.17	0.59
2:P:381:SER:OG	2:P:382:THR:N	2.29	0.59
1:K:11:GLN:HG2	1:K:74:VAL:HG21	1.84	0.59
2:F:306:ASP:OD1	2:F:306:ASP:C	2.40	0.58
1:I:290:GLU:HA	1:I:290:GLU:OE1	2.03	0.58
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.03	0.58
1:O:290:GLU:OE1	1:O:290:GLU:HA	2.04	0.58
1:C:290:GLU:OE1	1:C:290:GLU:HA	2.03	0.58
2:L:306:ASP:OD1	2:L:306:ASP:C	2.40	0.58
1:M:290:GLU:OE1	1:M:290:GLU:HA	2.03	0.58
1:G:290:GLU:HA	1:G:290:GLU:OE1	2.03	0.58
2:F:345:GLU:H	2:F:345:GLU:CD	2.10	0.58
1:G:262:TYR:HB3	1:G:263:PRO:HD2	1.86	0.58
2:L:345:GLU:H	2:L:345:GLU:CD	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:262:TYR:HB3	1:M:263:PRO:HD2	1.86	0.58
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.86	0.57
2:R:345:GLU:H	2:R:345:GLU:CD	2.10	0.57
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.86	0.57
1:I:262:TYR:HB3	1:I:263:PRO:HD2	1.86	0.57
1:O:262:TYR:HB3	1:O:263:PRO:HD2	1.86	0.57
1:E:262:TYR:HB3	1:E:263:PRO:HD2	1.86	0.57
1:K:262:TYR:HB3	1:K:263:PRO:HD2	1.86	0.57
1:K:290:GLU:OE1	1:K:290:GLU:HA	2.03	0.57
1:Q:262:TYR:HB3	1:Q:263:PRO:HD2	1.86	0.57
1:Q:290:GLU:HA	1:Q:290:GLU:OE1	2.03	0.57
1:E:290:GLU:HA	1:E:290:GLU:OE1	2.04	0.57
2:J:345:GLU:H	2:J:345:GLU:CD	2.10	0.56
2:B:345:GLU:H	2:B:345:GLU:CD	2.10	0.56
2:P:345:GLU:H	2:P:345:GLU:CD	2.10	0.56
2:P:228:ASN:ND2	5:P:901:GDP:HN1	1.98	0.55
2:B:228:ASN:ND2	5:B:901:GDP:HN1	1.98	0.55
2:J:228:ASN:ND2	5:J:901:GDP:HN1	1.98	0.55
2:H:345:GLU:H	2:H:345:GLU:CD	2.10	0.54
2:D:345:GLU:H	2:D:345:GLU:CD	2.10	0.53
2:N:345:GLU:H	2:N:345:GLU:CD	2.10	0.53
1:O:388:TRP:HA	1:O:388:TRP:CE3	2.44	0.53
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.44	0.53
1:M:216:ASN:HB3	1:M:275:VAL:O	2.09	0.53
2:R:228:ASN:ND2	5:R:901:GDP:HN1	1.98	0.53
1:C:216:ASN:HB3	1:C:275:VAL:O	2.09	0.53
1:G:216:ASN:HB3	1:G:275:VAL:O	2.09	0.53
1:G:388:TRP:HA	1:G:388:TRP:CE3	2.44	0.53
1:I:388:TRP:HA	1:I:388:TRP:CE3	2.44	0.53
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.44	0.53
1:E:388:TRP:HA	1:E:388:TRP:CE3	2.44	0.53
1:Q:388:TRP:HA	1:Q:388:TRP:CE3	2.44	0.53
1:K:388:TRP:CE3	1:K:388:TRP:HA	2.44	0.53
2:F:228:ASN:ND2	5:F:901:GDP:HN1	1.98	0.52
1:G:271:THR:OG1	1:G:301:GLN:NE2	2.42	0.52
2:P:306:ASP:OD1	2:P:308:ARG:HG2	2.09	0.52
2:B:306:ASP:OD1	2:B:308:ARG:HG2	2.10	0.52
1:C:271:THR:OG1	1:C:301:GLN:NE2	2.42	0.52
2:H:221:THR:H	2:H:222:PRO:HD3	1.73	0.52
2:J:306:ASP:OD1	2:J:308:ARG:HG2	2.10	0.52
1:M:388:TRP:HA	1:M:388:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:221:THR:H	2:N:222:PRO:HD3	1.73	0.52
2:D:221:THR:H	2:D:222:PRO:HD3	1.73	0.52
1:M:271:THR:OG1	1:M:301:GLN:NE2	2.42	0.52
1:Q:271:THR:OG1	1:Q:301:GLN:NE2	2.42	0.52
1:E:271:THR:OG1	1:E:301:GLN:NE2	2.42	0.52
2:H:221:THR:N	2:H:222:PRO:CD	2.73	0.52
2:H:306:ASP:OD1	2:H:308:ARG:HG2	2.10	0.52
1:K:216:ASN:HB3	1:K:275:VAL:O	2.09	0.52
2:L:221:THR:H	2:L:222:PRO:HD3	1.73	0.52
2:L:228:ASN:ND2	5:L:901:GDP:HN1	1.98	0.52
2:D:221:THR:N	2:D:222:PRO:CD	2.73	0.52
2:D:306:ASP:OD1	2:D:308:ARG:HG2	2.10	0.52
2:F:10:GLY:HA2	2:F:145:THR:OG1	2.10	0.52
1:K:271:THR:OG1	1:K:301:GLN:NE2	2.42	0.52
2:N:306:ASP:OD1	2:N:308:ARG:HG2	2.10	0.52
1:Q:216:ASN:HB3	1:Q:275:VAL:O	2.09	0.52
2:R:10:GLY:HA2	2:R:145:THR:OG1	2.10	0.52
1:E:216:ASN:HB3	1:E:275:VAL:O	2.09	0.52
2:F:221:THR:H	2:F:222:PRO:HD3	1.73	0.52
2:H:10:GLY:HA2	2:H:145:THR:OG1	2.10	0.52
2:L:10:GLY:HA2	2:L:145:THR:OG1	2.10	0.52
2:N:221:THR:N	2:N:222:PRO:CD	2.73	0.52
2:D:10:GLY:HA2	2:D:145:THR:OG1	2.10	0.52
2:N:10:GLY:HA2	2:N:145:THR:OG1	2.10	0.52
1:O:216:ASN:HB3	1:O:275:VAL:O	2.09	0.52
2:R:221:THR:N	2:R:222:PRO:CD	2.73	0.52
2:R:221:THR:H	2:R:222:PRO:HD3	1.73	0.52
1:A:216:ASN:HB3	1:A:275:VAL:O	2.09	0.51
1:I:216:ASN:HB3	1:I:275:VAL:O	2.09	0.51
2:F:390:ARG:HA	2:F:390:ARG:NE	2.26	0.51
2:B:390:ARG:HA	2:B:390:ARG:NE	2.26	0.51
2:H:390:ARG:HA	2:H:390:ARG:NE	2.26	0.51
2:J:390:ARG:HA	2:J:390:ARG:NE	2.26	0.51
2:L:390:ARG:NE	2:L:390:ARG:HA	2.26	0.51
2:P:10:GLY:HA2	2:P:145:THR:OG1	2.10	0.51
2:P:390:ARG:HA	2:P:390:ARG:NE	2.26	0.51
2:R:390:ARG:HA	2:R:390:ARG:NE	2.26	0.51
1:O:388:TRP:HA	1:O:388:TRP:HE3	1.74	0.51
2:B:10:GLY:HA2	2:B:145:THR:OG1	2.10	0.51
2:D:390:ARG:HA	2:D:390:ARG:NE	2.26	0.51
2:J:10:GLY:HA2	2:J:145:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:221:THR:H	2:P:222:PRO:HD3	1.73	0.51
1:Q:388:TRP:HA	1:Q:388:TRP:HE3	1.74	0.51
1:A:271:THR:OG1	1:A:301:GLN:NE2	2.42	0.51
2:B:221:THR:H	2:B:222:PRO:HD3	1.73	0.51
1:I:271:THR:OG1	1:I:301:GLN:NE2	2.42	0.51
1:K:237:SER:O	1:K:241:SER:OG	2.29	0.51
2:N:390:ARG:HA	2:N:390:ARG:NE	2.26	0.51
1:O:271:THR:OG1	1:O:301:GLN:NE2	2.42	0.51
1:Q:237:SER:O	1:Q:241:SER:OG	2.29	0.51
2:R:306:ASP:OD1	2:R:308:ARG:HG2	2.09	0.51
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.74	0.51
1:E:237:SER:O	1:E:241:SER:OG	2.29	0.51
2:F:306:ASP:OD1	2:F:308:ARG:HG2	2.10	0.51
2:J:221:THR:H	2:J:222:PRO:HD3	1.73	0.51
1:K:388:TRP:HA	1:K:388:TRP:HE3	1.74	0.51
2:L:306:ASP:OD1	2:L:308:ARG:HG2	2.10	0.51
1:E:388:TRP:HA	1:E:388:TRP:HE3	1.74	0.51
2:F:221:THR:N	2:F:222:PRO:CD	2.73	0.51
1:M:388:TRP:HA	1:M:388:TRP:HE3	1.74	0.51
1:C:388:TRP:HA	1:C:388:TRP:HE3	1.74	0.51
1:I:388:TRP:HA	1:I:388:TRP:HE3	1.74	0.51
2:J:221:THR:N	2:J:222:PRO:CD	2.73	0.51
1:A:237:SER:O	1:A:241:SER:OG	2.29	0.50
2:B:221:THR:N	2:B:222:PRO:CD	2.73	0.50
1:O:237:SER:O	1:O:241:SER:OG	2.29	0.50
1:I:237:SER:O	1:I:241:SER:OG	2.29	0.50
2:L:221:THR:N	2:L:222:PRO:CD	2.73	0.50
1:K:222:PRO:HG2	2:L:326:LYS:HB2	1.92	0.50
2:P:221:THR:N	2:P:222:PRO:CD	2.73	0.50
1:G:222:PRO:HG2	2:H:326:LYS:HB2	1.92	0.50
1:G:388:TRP:HA	1:G:388:TRP:HE3	1.74	0.50
3:G:501:GTP:O1A	2:H:254:LYS:NZ	2.42	0.50
1:I:222:PRO:HG2	2:J:326:LYS:HB2	1.92	0.50
3:M:501:GTP:O1A	2:N:254:LYS:NZ	2.42	0.50
3:C:501:GTP:O1A	2:D:254:LYS:NZ	2.42	0.50
1:E:222:PRO:HG2	2:F:326:LYS:HB2	1.92	0.50
1:A:222:PRO:HG2	2:B:326:LYS:HB2	1.92	0.50
2:H:2:ARG:N	2:H:131:CYS:O	2.45	0.50
2:N:2:ARG:N	2:N:131:CYS:O	2.45	0.50
1:Q:222:PRO:HG2	2:R:326:LYS:HB2	1.92	0.50
2:B:2:ARG:N	2:B:131:CYS:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PRO:HG2	2:D:326:LYS:HB2	1.92	0.50
2:D:2:ARG:N	2:D:131:CYS:O	2.45	0.50
1:G:237:SER:O	1:G:241:SER:OG	2.29	0.50
2:P:2:ARG:N	2:P:131:CYS:O	2.45	0.50
1:C:237:SER:O	1:C:241:SER:OG	2.29	0.50
2:F:2:ARG:N	2:F:131:CYS:O	2.45	0.50
2:J:2:ARG:N	2:J:131:CYS:O	2.45	0.50
1:M:222:PRO:HG2	2:N:326:LYS:HB2	1.92	0.50
1:M:237:SER:O	1:M:241:SER:OG	2.29	0.50
1:O:222:PRO:HG2	2:P:326:LYS:HB2	1.92	0.50
2:R:2:ARG:N	2:R:131:CYS:O	2.45	0.50
2:B:167:ASN:C	2:B:167:ASN:OD1	2.55	0.49
2:D:12:CYS:SG	2:D:13:GLY:N	2.85	0.49
2:F:167:ASN:OD1	2:F:167:ASN:C	2.56	0.49
2:H:12:CYS:SG	2:H:13:GLY:N	2.85	0.49
2:J:167:ASN:OD1	2:J:167:ASN:C	2.56	0.49
2:L:2:ARG:N	2:L:131:CYS:O	2.45	0.49
2:N:12:CYS:SG	2:N:13:GLY:N	2.85	0.49
2:N:167:ASN:C	2:N:167:ASN:OD1	2.55	0.49
2:P:167:ASN:OD1	2:P:167:ASN:C	2.56	0.49
2:D:167:ASN:C	2:D:167:ASN:OD1	2.56	0.49
2:H:167:ASN:OD1	2:H:167:ASN:C	2.56	0.49
2:L:12:CYS:SG	2:L:13:GLY:N	2.85	0.49
2:L:167:ASN:C	2:L:167:ASN:OD1	2.56	0.49
2:P:284:ARG:NH2	2:R:90:ASP:OD2	2.44	0.49
2:R:12:CYS:SG	2:R:13:GLY:N	2.85	0.49
2:R:167:ASN:OD1	2:R:167:ASN:C	2.56	0.49
2:F:12:CYS:SG	2:F:13:GLY:N	2.85	0.49
2:J:12:CYS:SG	2:J:13:GLY:N	2.85	0.49
3:O:501:GTP:O1A	2:P:254:LYS:NZ	2.42	0.49
3:A:501:GTP:O1A	2:B:254:LYS:NZ	2.42	0.49
3:I:501:GTP:O1A	2:J:254:LYS:NZ	2.42	0.49
2:B:12:CYS:SG	2:B:13:GLY:N	2.85	0.49
2:P:12:CYS:SG	2:P:13:GLY:N	2.85	0.49
2:P:96:GLN:NE2	2:P:96:GLN:O	2.46	0.49
2:B:96:GLN:O	2:B:96:GLN:NE2	2.46	0.49
3:E:501:GTP:O1A	2:F:254:LYS:NZ	2.42	0.49
3:K:501:GTP:O1A	2:L:254:LYS:NZ	2.42	0.49
2:R:96:GLN:O	2:R:96:GLN:NE2	2.46	0.49
2:F:96:GLN:O	2:F:96:GLN:NE2	2.46	0.49
2:N:96:GLN:O	2:N:96:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:501:GTP:O1A	2:R:254:LYS:NZ	2.42	0.49
2:D:96:GLN:O	2:D:96:GLN:NE2	2.46	0.48
2:J:96:GLN:O	2:J:96:GLN:NE2	2.46	0.48
2:L:96:GLN:O	2:L:96:GLN:NE2	2.46	0.48
2:H:96:GLN:O	2:H:96:GLN:NE2	2.46	0.48
1:K:220:GLU:OE1	2:L:326:LYS:NZ	2.43	0.47
1:E:220:GLU:OE1	2:F:326:LYS:NZ	2.43	0.47
2:H:288:VAL:HB	2:H:327:GLU:HG2	1.96	0.47
2:J:288:VAL:HB	2:J:327:GLU:HG2	1.96	0.47
2:N:228:ASN:ND2	5:N:901:GDP:HN1	1.98	0.47
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.96	0.47
2:D:288:VAL:HB	2:D:327:GLU:HG2	1.96	0.47
2:D:228:ASN:ND2	5:D:901:GDP:HN1	1.98	0.47
2:N:288:VAL:HB	2:N:327:GLU:HG2	1.96	0.47
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.97	0.47
1:C:53:PHE:HB3	1:C:61:HIS:HB3	1.97	0.47
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.96	0.47
2:H:228:ASN:ND2	5:H:901:GDP:HN1	1.98	0.47
1:M:53:PHE:HB3	1:M:61:HIS:HB3	1.97	0.47
1:M:228:ASN:HD21	3:M:501:GTP:HN1	1.63	0.47
1:M:246:GLY:HA3	1:M:356:ASN:HA	1.97	0.47
1:O:53:PHE:HB3	1:O:61:HIS:HB3	1.97	0.47
2:P:288:VAL:HB	2:P:327:GLU:HG2	1.96	0.47
1:Q:53:PHE:HB3	1:Q:61:HIS:HB3	1.97	0.47
1:C:228:ASN:HD21	3:C:501:GTP:HN1	1.62	0.47
1:G:53:PHE:HB3	1:G:61:HIS:HB3	1.97	0.47
1:G:246:GLY:HA3	1:G:356:ASN:HA	1.96	0.47
1:I:53:PHE:HB3	1:I:61:HIS:HB3	1.97	0.47
1:E:53:PHE:HB3	1:E:61:HIS:HB3	1.97	0.47
1:G:228:ASN:HD21	3:G:501:GTP:HN1	1.62	0.47
1:K:53:PHE:HB3	1:K:61:HIS:HB3	1.97	0.47
2:L:288:VAL:HB	2:L:327:GLU:HG2	1.96	0.47
1:O:228:ASN:HD21	3:O:501:GTP:HN1	1.63	0.47
1:Q:228:ASN:HD21	3:Q:501:GTP:HN1	1.63	0.47
2:R:288:VAL:HB	2:R:327:GLU:HG2	1.96	0.47
1:A:228:ASN:HD21	3:A:501:GTP:HN1	1.63	0.46
1:E:325:PRO:HB2	2:R:210:TYR:OH	2.15	0.46
2:F:288:VAL:HB	2:F:327:GLU:HG2	1.96	0.46
2:N:142:GLY:HA3	2:N:183:GLU:HG3	1.97	0.46
2:P:142:GLY:HA3	2:P:183:GLU:HG3	1.97	0.46
2:B:142:GLY:HA3	2:B:183:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:ASN:HD21	3:E:501:GTP:HN1	1.63	0.46
1:Q:255:PHE:HD1	1:Q:255:PHE:HA	1.54	0.46
1:A:243:ARG:HA	1:A:243:ARG:HE	1.81	0.46
1:C:243:ARG:HA	1:C:243:ARG:HE	1.81	0.46
2:D:142:GLY:HA3	2:D:183:GLU:HG3	1.97	0.46
1:G:243:ARG:HA	1:G:243:ARG:HE	1.81	0.46
1:I:228:ASN:HD21	3:I:501:GTP:HN1	1.63	0.46
1:I:243:ARG:HA	1:I:243:ARG:HE	1.81	0.46
2:H:142:GLY:HA3	2:H:183:GLU:HG3	1.97	0.46
2:J:142:GLY:HA3	2:J:183:GLU:HG3	1.97	0.46
1:K:332:ILE:HA	1:K:335:ILE:HG12	1.97	0.46
1:M:243:ARG:HA	1:M:243:ARG:HE	1.81	0.46
1:O:243:ARG:HA	1:O:243:ARG:HE	1.81	0.46
1:O:246:GLY:HA3	1:O:356:ASN:HA	1.96	0.46
2:R:103:TRP:CD1	2:R:103:TRP:C	2.94	0.46
1:E:255:PHE:HD1	1:E:255:PHE:HA	1.54	0.46
1:E:332:ILE:HA	1:E:335:ILE:HG12	1.97	0.46
2:F:103:TRP:CD1	2:F:103:TRP:C	2.94	0.46
1:K:228:ASN:HD21	3:K:501:GTP:HN1	1.63	0.46
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	1.96	0.46
1:I:332:ILE:HA	1:I:335:ILE:HG12	1.97	0.46
1:K:246:GLY:HA3	1:K:356:ASN:HA	1.97	0.46
2:L:103:TRP:CD1	2:L:103:TRP:C	2.94	0.46
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.97	0.46
1:E:246:GLY:HA3	1:E:356:ASN:HA	1.96	0.46
1:G:190:THR:OG1	1:G:191:THR:N	2.49	0.46
1:I:283:HIS:HA	1:K:56:THR:HG21	1.96	0.46
1:Q:332:ILE:HA	1:Q:335:ILE:HG12	1.97	0.46
1:A:332:ILE:HA	1:A:335:ILE:HG12	1.97	0.46
1:I:246:GLY:HA3	1:I:356:ASN:HA	1.96	0.46
1:K:255:PHE:HD1	1:K:255:PHE:HA	1.54	0.46
2:R:142:GLY:HA3	2:R:183:GLU:HG3	1.97	0.46
1:C:190:THR:OG1	1:C:191:THR:N	2.49	0.46
2:F:142:GLY:HA3	2:F:183:GLU:HG3	1.97	0.46
1:O:332:ILE:HA	1:O:335:ILE:HG12	1.97	0.46
2:P:103:TRP:CD1	2:P:103:TRP:C	2.94	0.46
2:B:103:TRP:CD1	2:B:103:TRP:C	2.94	0.45
2:L:142:GLY:HA3	2:L:183:GLU:HG3	1.97	0.45
1:M:190:THR:OG1	1:M:191:THR:N	2.49	0.45
2:N:28:HIS:NE2	2:N:243:ARG:NH1	2.65	0.45
2:N:284:ARG:NH2	2:P:90:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HB2	2:B:254:LYS:HE3	1.99	0.45
2:D:28:HIS:NE2	2:D:243:ARG:NH1	2.65	0.45
1:E:101:ASN:HB2	2:F:254:LYS:HE3	1.98	0.45
2:H:28:HIS:NE2	2:H:243:ARG:NH1	2.65	0.45
1:I:101:ASN:HB2	2:J:254:LYS:HE3	1.99	0.45
1:K:101:ASN:HB2	2:L:254:LYS:HE3	1.99	0.45
1:K:190:THR:OG1	1:K:191:THR:N	2.49	0.45
1:O:220:GLU:OE1	2:P:326:LYS:NZ	2.43	0.45
2:R:28:HIS:NE2	2:R:243:ARG:NH1	2.65	0.45
1:C:101:ASN:HB2	2:D:254:LYS:HE3	1.99	0.45
1:G:101:ASN:HB2	2:H:254:LYS:HE3	1.99	0.45
1:M:101:ASN:HB2	2:N:254:LYS:HE3	1.99	0.45
1:E:190:THR:OG1	1:E:191:THR:N	2.49	0.45
2:F:28:HIS:NE2	2:F:243:ARG:NH1	2.65	0.45
2:J:103:TRP:CD1	2:J:103:TRP:C	2.94	0.45
2:J:331:GLN:OE1	2:J:331:GLN:HA	2.17	0.45
1:O:101:ASN:HB2	2:P:254:LYS:HE3	1.99	0.45
1:Q:101:ASN:HB2	2:R:254:LYS:HE3	1.99	0.45
2:R:139:HIS:O	2:R:170:SER:HA	2.17	0.45
2:B:28:HIS:NE2	2:B:243:ARG:NH1	2.65	0.45
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.45
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.17	0.45
2:F:139:HIS:O	2:F:170:SER:HA	2.16	0.45
2:H:331:GLN:OE1	2:H:331:GLN:HA	2.17	0.45
2:J:28:HIS:NE2	2:J:243:ARG:NH1	2.65	0.45
2:L:28:HIS:NE2	2:L:243:ARG:NH1	2.65	0.45
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.50	0.45
1:M:221:ARG:N	1:M:222:PRO:CD	2.80	0.45
1:M:313:MET:SD	1:M:435:VAL:HG11	2.57	0.45
2:N:331:GLN:OE1	2:N:331:GLN:HA	2.17	0.45
2:P:139:HIS:O	2:P:170:SER:HA	2.17	0.45
1:C:221:ARG:N	1:C:222:PRO:CD	2.80	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.57	0.45
2:P:28:HIS:NE2	2:P:243:ARG:NH1	2.65	0.45
2:P:389:LYS:NZ	2:P:393:GLU:OE2	2.44	0.45
1:Q:190:THR:OG1	1:Q:191:THR:N	2.49	0.45
1:Q:313:MET:SD	1:Q:435:VAL:HG11	2.57	0.45
2:B:331:GLN:OE1	2:B:331:GLN:HA	2.17	0.45
2:J:139:HIS:O	2:J:170:SER:HA	2.17	0.45
1:O:313:MET:SD	1:O:435:VAL:HG11	2.57	0.45
2:P:331:GLN:HA	2:P:331:GLN:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:SD	1:A:435:VAL:HG11	2.57	0.45
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.50	0.45
1:E:313:MET:SD	1:E:435:VAL:HG11	2.57	0.45
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.50	0.45
1:G:313:MET:SD	1:G:435:VAL:HG11	2.57	0.45
1:I:221:ARG:N	1:I:222:PRO:CD	2.80	0.45
1:I:313:MET:SD	1:I:435:VAL:HG11	2.57	0.45
2:L:139:HIS:O	2:L:170:SER:HA	2.17	0.45
1:M:332:ILE:HA	1:M:335:ILE:HG12	1.97	0.45
2:P:262:PHE:HA	2:P:263:PRO:HD3	1.90	0.45
1:A:221:ARG:N	1:A:222:PRO:CD	2.80	0.44
1:C:332:ILE:HA	1:C:335:ILE:HG12	1.97	0.44
1:G:332:ILE:HA	1:G:335:ILE:HG12	1.97	0.44
1:K:313:MET:SD	1:K:435:VAL:HG11	2.57	0.44
1:G:221:ARG:N	1:G:222:PRO:CD	2.80	0.44
1:G:283:HIS:HA	1:I:56:THR:HG21	2.00	0.44
2:H:61:TYR:CD1	2:H:61:TYR:N	2.86	0.44
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.17	0.44
2:N:61:TYR:CD1	2:N:61:TYR:N	2.86	0.44
2:N:139:HIS:O	2:N:170:SER:HA	2.17	0.44
1:O:221:ARG:N	1:O:222:PRO:CD	2.80	0.44
2:D:61:TYR:CD1	2:D:61:TYR:N	2.86	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.17	0.44
2:N:103:TRP:CD1	2:N:103:TRP:C	2.94	0.44
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.50	0.44
2:F:331:GLN:HA	2:F:331:GLN:OE1	2.17	0.44
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.50	0.44
2:N:262:PHE:HA	2:N:263:PRO:HD3	1.90	0.44
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.50	0.44
2:P:61:TYR:CD1	2:P:61:TYR:N	2.86	0.44
2:B:61:TYR:CD1	2:B:61:TYR:N	2.86	0.44
2:B:242:LEU:N	2:B:242:LEU:CD1	2.81	0.44
2:D:103:TRP:CD1	2:D:103:TRP:C	2.94	0.44
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.50	0.44
2:H:139:HIS:O	2:H:170:SER:HA	2.17	0.44
2:R:242:LEU:CD1	2:R:242:LEU:N	2.81	0.44
2:R:331:GLN:HA	2:R:331:GLN:OE1	2.17	0.44
2:F:242:LEU:N	2:F:242:LEU:CD1	2.81	0.44
2:J:61:TYR:CD1	2:J:61:TYR:N	2.86	0.44
2:J:242:LEU:CD1	2:J:242:LEU:N	2.81	0.44
2:L:74:THR:OG1	2:L:75:MET:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:242:LEU:N	2:P:242:LEU:CD1	2.81	0.44
1:C:325:PRO:HB2	2:N:210:TYR:OH	2.18	0.44
2:F:74:THR:OG1	2:F:75:MET:N	2.51	0.44
2:H:74:THR:OG1	2:H:75:MET:N	2.51	0.44
2:L:242:LEU:CD1	2:L:242:LEU:N	2.81	0.44
1:M:100:ALA:O	1:M:101:ASN:HB3	2.18	0.44
2:N:248:LEU:HD23	2:N:248:LEU:HA	1.80	0.44
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.50	0.44
2:D:74:THR:OG1	2:D:75:MET:N	2.51	0.43
2:H:103:TRP:CD1	2:H:103:TRP:C	2.94	0.43
2:N:74:THR:OG1	2:N:75:MET:N	2.51	0.43
2:R:74:THR:OG1	2:R:75:MET:N	2.51	0.43
1:C:100:ALA:O	1:C:101:ASN:HB3	2.18	0.43
1:E:30:ILE:HG12	1:E:36:MET:SD	2.58	0.43
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.50	0.43
1:K:30:ILE:HG12	1:K:36:MET:SD	2.58	0.43
1:M:63:PRO:O	1:M:91:GLN:NE2	2.50	0.43
1:O:100:ALA:O	1:O:101:ASN:HB3	2.18	0.43
1:Q:221:ARG:N	1:Q:222:PRO:CD	2.80	0.43
1:A:100:ALA:O	1:A:101:ASN:HB3	2.18	0.43
1:C:63:PRO:O	1:C:91:GLN:NE2	2.50	0.43
1:G:100:ALA:O	1:G:101:ASN:HB3	2.18	0.43
1:K:221:ARG:N	1:K:222:PRO:CD	2.80	0.43
1:Q:30:ILE:HG12	1:Q:36:MET:SD	2.58	0.43
1:E:221:ARG:N	1:E:222:PRO:CD	2.80	0.43
1:G:30:ILE:HG12	1:G:36:MET:SD	2.58	0.43
1:G:63:PRO:O	1:G:91:GLN:NE2	2.50	0.43
2:R:61:TYR:CD1	2:R:61:TYR:N	2.86	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.58	0.43
2:F:61:TYR:CD1	2:F:61:TYR:N	2.86	0.43
1:I:100:ALA:O	1:I:101:ASN:HB3	2.18	0.43
2:L:61:TYR:CD1	2:L:61:TYR:N	2.86	0.43
1:O:30:ILE:HG12	1:O:36:MET:SD	2.58	0.43
1:O:190:THR:OG1	1:O:191:THR:N	2.49	0.43
1:A:30:ILE:HG12	1:A:36:MET:SD	2.58	0.43
1:C:297:GLU:HA	1:C:298:PRO:HD3	1.89	0.43
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.43
2:J:183:GLU:N	2:J:184:PRO:CD	2.82	0.43
2:L:248:LEU:HD23	2:L:248:LEU:HA	1.80	0.43
2:N:109:THR:OG1	2:N:110:GLU:N	2.51	0.43
2:P:109:THR:OG1	2:P:110:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:OG1	1:A:191:THR:N	2.49	0.43
1:A:325:PRO:HB2	2:P:210:TYR:OH	2.19	0.43
2:B:109:THR:OG1	2:B:110:GLU:N	2.51	0.43
1:C:346:TRP:HB3	2:N:401:ARG:HG3	2.00	0.43
2:H:109:THR:OG1	2:H:110:GLU:N	2.51	0.43
2:J:109:THR:OG1	2:J:110:GLU:N	2.51	0.43
1:M:30:ILE:HG12	1:M:36:MET:SD	2.58	0.43
2:N:242:LEU:N	2:N:242:LEU:CD1	2.81	0.43
2:R:109:THR:OG1	2:R:110:GLU:N	2.51	0.43
2:B:183:GLU:N	2:B:184:PRO:CD	2.82	0.43
2:D:242:LEU:N	2:D:242:LEU:CD1	2.81	0.43
2:F:109:THR:OG1	2:F:110:GLU:N	2.51	0.43
1:I:190:THR:OG1	1:I:191:THR:N	2.49	0.43
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.80	0.43
1:I:30:ILE:HG12	1:I:36:MET:SD	2.58	0.43
2:L:109:THR:OG1	2:L:110:GLU:N	2.51	0.43
2:N:183:GLU:N	2:N:184:PRO:CD	2.82	0.43
2:P:183:GLU:N	2:P:184:PRO:CD	2.82	0.43
2:D:183:GLU:N	2:D:184:PRO:CD	2.82	0.43
2:H:242:LEU:N	2:H:242:LEU:CD1	2.81	0.43
1:G:297:GLU:HA	1:G:298:PRO:HD3	1.89	0.42
1:O:63:PRO:O	1:O:91:GLN:NE2	2.50	0.42
2:H:183:GLU:N	2:H:184:PRO:CD	2.82	0.42
2:J:74:THR:OG1	2:J:75:MET:N	2.51	0.42
2:L:332:MET:HA	2:L:332:MET:CE	2.46	0.42
1:A:63:PRO:O	1:A:91:GLN:NE2	2.50	0.42
1:K:254:GLU:HA	1:K:257:THR:OG1	2.20	0.42
1:Q:254:GLU:HA	1:Q:257:THR:OG1	2.20	0.42
1:A:254:GLU:HA	1:A:257:THR:OG1	2.20	0.42
2:B:74:THR:OG1	2:B:75:MET:N	2.51	0.42
1:E:254:GLU:HA	1:E:257:THR:OG1	2.20	0.42
2:F:183:GLU:N	2:F:184:PRO:CD	2.82	0.42
2:F:332:MET:HA	2:F:332:MET:CE	2.46	0.42
2:H:248:LEU:HD23	2:H:248:LEU:HA	1.80	0.42
1:I:254:GLU:HA	1:I:257:THR:OG1	2.20	0.42
2:L:183:GLU:N	2:L:184:PRO:CD	2.82	0.42
1:O:254:GLU:HA	1:O:257:THR:OG1	2.20	0.42
1:C:254:GLU:HA	1:C:257:THR:OG1	2.20	0.42
1:I:63:PRO:O	1:I:91:GLN:NE2	2.50	0.42
1:K:147:SER:HB2	1:K:190:THR:HG21	2.01	0.42
1:Q:347:CYS:HA	1:Q:348:PRO:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:183:GLU:N	2:R:184:PRO:CD	2.82	0.42
1:A:346:TRP:HB3	2:P:401:ARG:HG3	2.01	0.42
2:D:408:TYR:N	2:D:408:TYR:CD1	2.87	0.42
1:G:254:GLU:HA	1:G:257:THR:OG1	2.20	0.42
2:H:408:TYR:N	2:H:408:TYR:CD1	2.87	0.42
1:M:254:GLU:HA	1:M:257:THR:OG1	2.20	0.42
2:P:338:LYS:NZ	2:R:127:GLU:OE1	2.52	0.42
2:R:332:MET:HA	2:R:332:MET:CE	2.46	0.42
2:B:408:TYR:CD1	2:B:408:TYR:N	2.87	0.42
2:F:408:TYR:N	2:F:408:TYR:CD1	2.88	0.42
1:K:100:ALA:O	1:K:101:ASN:HB3	2.18	0.42
2:L:408:TYR:CD1	2:L:408:TYR:N	2.87	0.42
1:M:255:PHE:HD1	1:M:255:PHE:HA	1.54	0.42
2:N:408:TYR:N	2:N:408:TYR:CD1	2.87	0.42
2:P:74:THR:OG1	2:P:75:MET:N	2.51	0.42
2:P:408:TYR:N	2:P:408:TYR:CD1	2.87	0.42
1:Q:326:LYS:HB3	1:Q:326:LYS:HE3	1.84	0.42
2:R:408:TYR:CD1	2:R:408:TYR:N	2.87	0.42
1:E:147:SER:HB2	1:E:190:THR:HG21	2.01	0.42
2:J:408:TYR:CD1	2:J:408:TYR:N	2.88	0.42
1:Q:147:SER:HB2	1:Q:190:THR:HG21	2.01	0.42
1:Q:358:GLU:HA	1:Q:359:PRO:HD2	1.90	0.42
1:C:255:PHE:HD1	1:C:255:PHE:HA	1.54	0.42
1:E:347:CYS:HA	1:E:348:PRO:HD2	1.87	0.42
1:E:352:LYS:HD2	2:R:179:ASP:HB3	2.01	0.42
1:G:147:SER:HB2	1:G:190:THR:HG21	2.01	0.42
1:G:211:ASP:HA	1:G:214:ARG:HG2	2.02	0.42
1:I:147:SER:HB2	1:I:190:THR:HG21	2.01	0.42
1:C:211:ASP:HA	1:C:214:ARG:HG2	2.02	0.42
1:E:100:ALA:O	1:E:101:ASN:HB3	2.18	0.42
1:Q:63:PRO:O	1:Q:91:GLN:NE2	2.50	0.42
1:A:147:SER:HB2	1:A:190:THR:HG21	2.01	0.41
1:E:326:LYS:HB3	1:E:326:LYS:HE3	1.84	0.41
1:I:211:ASP:HA	1:I:214:ARG:HG2	2.02	0.41
1:K:147:SER:HB2	1:K:190:THR:CG2	2.50	0.41
1:K:347:CYS:HA	1:K:348:PRO:HD2	1.87	0.41
1:M:211:ASP:HA	1:M:214:ARG:HG2	2.02	0.41
1:O:211:ASP:HA	1:O:214:ARG:HG2	2.02	0.41
1:A:211:ASP:HA	1:A:214:ARG:HG2	2.02	0.41
1:C:147:SER:HB2	1:C:190:THR:HG21	2.01	0.41
1:E:63:PRO:O	1:E:91:GLN:NE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:PRO:O	1:K:91:GLN:NE2	2.50	0.41
1:Q:100:ALA:O	1:Q:101:ASN:HB3	2.18	0.41
1:E:147:SER:HB2	1:E:190:THR:CG2	2.50	0.41
1:E:211:ASP:HA	1:E:214:ARG:HG2	2.02	0.41
1:G:147:SER:HB2	1:G:190:THR:CG2	2.50	0.41
1:G:255:PHE:HD1	1:G:255:PHE:HA	1.54	0.41
1:I:147:SER:HB2	1:I:190:THR:CG2	2.50	0.41
1:K:211:ASP:HA	1:K:214:ARG:HG2	2.02	0.41
1:Q:211:ASP:HA	1:Q:214:ARG:HG2	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:CG2	2.50	0.41
1:C:147:SER:HB2	1:C:190:THR:CG2	2.50	0.41
1:G:166:LYS:NZ	1:G:199:ASP:OD2	2.49	0.41
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.69	0.41
1:I:133:GLN:NE2	1:I:133:GLN:HA	2.36	0.41
1:M:147:SER:HB2	1:M:190:THR:CG2	2.50	0.41
1:M:220:GLU:OE1	2:N:326:LYS:NZ	2.43	0.41
1:Q:147:SER:HB2	1:Q:190:THR:CG2	2.50	0.41
1:A:133:GLN:NE2	1:A:133:GLN:HA	2.36	0.41
1:C:133:GLN:NE2	1:C:133:GLN:HA	2.35	0.41
1:C:166:LYS:NZ	1:C:199:ASP:OD2	2.49	0.41
1:E:133:GLN:NE2	1:E:133:GLN:HA	2.35	0.41
1:G:133:GLN:NE2	1:G:133:GLN:HA	2.36	0.41
1:K:133:GLN:NE2	1:K:133:GLN:HA	2.36	0.41
1:K:326:LYS:HB3	1:K:326:LYS:HE3	1.84	0.41
1:M:147:SER:HB2	1:M:190:THR:HG21	2.01	0.41
1:O:147:SER:HB2	1:O:190:THR:CG2	2.50	0.41
1:O:147:SER:HB2	1:O:190:THR:HG21	2.01	0.41
1:C:220:GLU:OE1	2:D:326:LYS:NZ	2.43	0.41
1:E:163:LYS:NZ	2:R:411:GLU:OE2	2.48	0.41
2:H:88:ARG:HA	2:H:89:PRO:HD3	1.86	0.41
1:M:133:GLN:NE2	1:M:133:GLN:HA	2.36	0.41
1:M:166:LYS:NZ	1:M:199:ASP:OD2	2.49	0.41
1:O:133:GLN:NE2	1:O:133:GLN:HA	2.36	0.41
1:A:220:GLU:OE1	2:B:326:LYS:NZ	2.43	0.41
1:E:388:TRP:CE3	1:E:388:TRP:CA	3.04	0.41
1:Q:133:GLN:NE2	1:Q:133:GLN:HA	2.36	0.41
1:A:388:TRP:CE3	1:A:388:TRP:CA	3.04	0.41
2:B:332:MET:HA	2:B:332:MET:CE	2.46	0.41
2:D:181:VAL:HG11	1:G:346:TRP:CZ3	2.56	0.41
1:G:220:GLU:OE1	2:H:326:LYS:NZ	2.43	0.41
1:G:388:TRP:CE3	1:G:388:TRP:CA	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:TRP:CE3	1:K:388:TRP:CA	3.04	0.41
1:Q:388:TRP:CE3	1:Q:388:TRP:CA	3.04	0.41
1:C:388:TRP:CE3	1:C:388:TRP:CA	3.04	0.41
1:G:363:VAL:HA	1:G:364:PRO:HD3	1.92	0.41
1:I:388:TRP:CE3	1:I:388:TRP:CA	3.04	0.41
1:O:90:GLU:OE2	1:O:121:ARG:NH1	2.54	0.41
1:O:388:TRP:CE3	1:O:388:TRP:CA	3.04	0.41
1:Q:297:GLU:HA	1:Q:298:PRO:HD3	1.89	0.41
2:R:389:LYS:NZ	2:R:393:GLU:OE2	2.44	0.41
1:A:90:GLU:OE2	1:A:121:ARG:NH1	2.54	0.41
1:A:166:LYS:NZ	1:A:199:ASP:OD2	2.49	0.41
1:C:363:VAL:HA	1:C:364:PRO:HD3	1.92	0.41
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.69	0.41
2:D:88:ARG:HA	2:D:89:PRO:HD3	1.86	0.41
2:F:401:ARG:O	2:F:402:LYS:HB2	2.21	0.41
1:I:90:GLU:OE2	1:I:121:ARG:NH1	2.54	0.41
1:I:166:LYS:NZ	1:I:199:ASP:OD2	2.49	0.41
2:L:401:ARG:O	2:L:402:LYS:HB2	2.21	0.41
1:M:388:TRP:CE3	1:M:388:TRP:CA	3.04	0.41
1:O:166:LYS:NZ	1:O:199:ASP:OD2	2.49	0.41
1:O:283:HIS:O	1:Q:88:HIS:HD2	2.04	0.41
2:P:248:LEU:HA	2:P:248:LEU:HD23	1.80	0.41
2:P:332:MET:HA	2:P:332:MET:CE	2.46	0.41
1:C:90:GLU:OE2	1:C:121:ARG:NH1	2.54	0.40
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.69	0.40
1:G:90:GLU:OE2	1:G:121:ARG:NH1	2.54	0.40
1:I:363:VAL:HA	1:I:364:PRO:HD3	1.92	0.40
1:O:435:VAL:O	1:O:435:VAL:HG12	2.18	0.40
1:C:345:ASP:OD2	1:C:439:SER:OG	2.35	0.40
1:M:90:GLU:OE2	1:M:121:ARG:NH1	2.54	0.40
1:M:363:VAL:HA	1:M:364:PRO:HD3	1.92	0.40
1:O:326:LYS:HB3	1:O:326:LYS:HE3	1.84	0.40
1:Q:402:ARG:HD3	1:Q:402:ARG:HA	1.69	0.40
2:R:401:ARG:O	2:R:402:LYS:HB2	2.21	0.40
1:E:166:LYS:NZ	1:E:199:ASP:OD2	2.49	0.40
1:E:297:GLU:HA	1:E:298:PRO:HD3	1.89	0.40
2:L:266:HIS:ND1	2:L:266:HIS:C	2.80	0.40
1:M:435:VAL:O	1:M:435:VAL:HG12	2.18	0.40
1:Q:166:LYS:NZ	1:Q:199:ASP:OD2	2.49	0.40
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.92	0.40
1:C:141:PHE:HB2	1:C:173:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ARG:HA	1:E:243:ARG:HE	1.81	0.40
1:M:154:MET:HE3	1:M:154:MET:HB3	1.93	0.40
1:Q:243:ARG:HA	1:Q:243:ARG:HE	1.81	0.40
1:A:435:VAL:O	1:A:435:VAL:HG12	2.18	0.40
2:F:266:HIS:ND1	2:F:266:HIS:C	2.80	0.40
1:G:141:PHE:HB2	1:G:173:PRO:HD3	2.04	0.40
1:I:141:PHE:HB2	1:I:173:PRO:HD3	2.04	0.40
1:K:297:GLU:HA	1:K:298:PRO:HD3	1.89	0.40
1:K:402:ARG:HD3	1:K:402:ARG:HA	1.69	0.40
1:M:141:PHE:HB2	1:M:173:PRO:HD3	2.04	0.40
1:M:345:ASP:OD2	1:M:439:SER:OG	2.35	0.40
2:R:266:HIS:ND1	2:R:266:HIS:C	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	C	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	E	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	G	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	I	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	K	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	M	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	O	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
1	Q	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	24	63
2	B	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	F	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	H	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	J	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	L	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	N	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	P	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
2	R	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	18	55
All	All	7632/7794 (98%)	7353 (96%)	234 (3%)	45 (1%)	23	58

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLY
2	D	98	GLY
2	F	98	GLY
2	H	98	GLY
2	J	98	GLY
2	L	98	GLY
2	N	98	GLY
2	P	98	GLY
2	R	98	GLY
1	A	345	ASP
1	C	345	ASP
1	E	345	ASP
1	K	345	ASP
2	B	350	ASN
2	D	350	ASN
2	F	350	ASN
1	G	345	ASP
2	H	350	ASN
1	I	345	ASP
2	J	350	ASN
2	L	350	ASN
1	M	345	ASP
2	N	350	ASN
1	O	345	ASP
2	P	350	ASN
1	Q	345	ASP

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Mol	Chain	Res	Type
2	R	350	ASN
1	A	349	THR
1	C	349	THR
1	E	349	THR
1	I	349	THR
1	M	349	THR
1	O	349	THR
1	Q	349	THR
1	G	349	THR
1	K	349	THR
2	B	221	THR
2	D	221	THR
2	F	221	THR
2	H	221	THR
2	J	221	THR
2	L	221	THR
2	N	221	THR
2	P	221	THR
2	R	221	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	C	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	E	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	G	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	I	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	K	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	M	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	O	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	Q	360/368 (98%)	359 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/368 (100%)	367 (100%)	0	100	100
2	D	367/368 (100%)	367 (100%)	0	100	100
2	F	367/368 (100%)	367 (100%)	0	100	100
2	H	367/368 (100%)	367 (100%)	0	100	100
2	J	367/368 (100%)	367 (100%)	0	100	100
2	L	367/368 (100%)	367 (100%)	0	100	100
2	N	367/368 (100%)	367 (100%)	0	100	100
2	P	367/368 (100%)	367 (100%)	0	100	100
2	R	367/368 (100%)	367 (100%)	0	100	100
All	All	6543/6624 (99%)	6534 (100%)	9 (0%)	87	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	PHE
1	C	255	PHE
1	E	255	PHE
1	G	255	PHE
1	I	255	PHE
1	K	255	PHE
1	M	255	PHE
1	O	255	PHE
1	Q	255	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	B	8	GLN
2	B	96	GLN
2	B	249	ASN
2	B	339	ASN
2	B	385	GLN
2	B	436	GLN
1	C	258	ASN
1	C	301	GLN
2	D	8	GLN
2	D	339	ASN

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Mol	Chain	Res	Type
2	D	385	GLN
2	D	436	GLN
1	E	283	HIS
1	E	301	GLN
2	F	8	GLN
2	F	96	GLN
2	F	385	GLN
2	F	436	GLN
1	G	258	ASN
1	G	301	GLN
2	H	8	GLN
2	H	11	GLN
2	H	96	GLN
2	H	339	ASN
2	H	385	GLN
2	H	436	GLN
1	I	258	ASN
1	I	301	GLN
2	J	8	GLN
2	J	11	GLN
2	J	96	GLN
2	J	249	ASN
2	J	282	GLN
2	J	339	ASN
2	J	385	GLN
2	J	436	GLN
1	K	258	ASN
1	K	283	HIS
1	K	301	GLN
2	L	8	GLN
2	L	11	GLN
2	L	96	GLN
2	L	339	ASN
2	L	385	GLN
2	L	436	GLN
1	M	216	ASN
1	M	258	ASN
1	M	301	GLN
2	N	8	GLN
2	N	59	ASN
2	N	96	GLN
2	N	339	ASN

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Mol	Chain	Res	Type
2	N	385	GLN
2	N	436	GLN
1	O	216	ASN
1	O	258	ASN
1	O	301	GLN
2	P	8	GLN
2	P	339	ASN
2	P	385	GLN
2	P	436	GLN
1	Q	258	ASN
1	Q	283	HIS
1	Q	301	GLN
2	R	8	GLN
2	R	249	ASN
2	R	385	GLN
2	R	436	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	M	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	G	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	Q	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	D	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	L	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	18 (40%)
5	GDP	H	901	-	29,30,30	2.96	11 (37%)	45,47,47	3.49	17 (37%)
3	GTP	O	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	A	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	E	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	B	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
3	GTP	K	501	4	33,34,34	1.91	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	I	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	J	901	-	29,30,30	2.97	12 (41%)	45,47,47	3.50	17 (37%)
5	GDP	N	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	P	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
3	GTP	C	501	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	F	901	-	29,30,30	2.97	12 (41%)	45,47,47	3.49	18 (40%)
5	GDP	R	901	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	M	501	4	-	4/22/38/38	0/3/3/3
3	GTP	G	501	4	-	4/22/38/38	0/3/3/3
3	GTP	Q	501	4	-	4/22/38/38	0/3/3/3
5	GDP	D	901	-	-	4/16/32/32	0/3/3/3
5	GDP	L	901	-	-	4/16/32/32	0/3/3/3
5	GDP	H	901	-	-	4/16/32/32	0/3/3/3
3	GTP	O	501	4	-	4/22/38/38	0/3/3/3
3	GTP	A	501	4	-	4/22/38/38	0/3/3/3
3	GTP	E	501	4	-	4/22/38/38	0/3/3/3
5	GDP	B	901	-	-	4/16/32/32	0/3/3/3
3	GTP	K	501	4	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	I	501	4	-	4/22/38/38	0/3/3/3
5	GDP	J	901	-	-	4/16/32/32	0/3/3/3
5	GDP	N	901	-	-	4/16/32/32	0/3/3/3
5	GDP	P	901	-	-	4/16/32/32	0/3/3/3
3	GTP	C	501	4	-	4/22/38/38	0/3/3/3
5	GDP	F	901	-	-	4/16/32/32	0/3/3/3
5	GDP	R	901	-	-	4/16/32/32	0/3/3/3

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	GDP	PA-O3A	7.57	1.67	1.59
5	H	901	GDP	PA-O3A	7.57	1.67	1.59
5	R	901	GDP	PA-O3A	7.54	1.67	1.59
5	J	901	GDP	PA-O3A	7.54	1.67	1.59
5	B	901	GDP	PA-O3A	7.54	1.67	1.59
5	N	901	GDP	PA-O3A	7.54	1.67	1.59
5	D	901	GDP	PA-O3A	7.52	1.67	1.59
5	L	901	GDP	PA-O3A	7.52	1.67	1.59
5	P	901	GDP	PA-O3A	7.47	1.67	1.59
3	C	501	GTP	PA-O3A	-6.12	1.52	1.59
3	Q	501	GTP	PA-O3A	-6.08	1.52	1.59
3	O	501	GTP	PA-O3A	-6.06	1.53	1.59
3	A	501	GTP	PA-O3A	-6.06	1.53	1.59
3	K	501	GTP	PA-O3A	-6.06	1.53	1.59
3	E	501	GTP	PA-O3A	-6.05	1.53	1.59
3	M	501	GTP	PA-O3A	-6.05	1.53	1.59
3	I	501	GTP	PA-O3A	-6.03	1.53	1.59
3	G	501	GTP	PA-O3A	-6.00	1.53	1.59
5	J	901	GDP	O6-C6	6.00	1.34	1.23
5	R	901	GDP	O6-C6	6.00	1.34	1.23
5	N	901	GDP	O6-C6	5.98	1.34	1.23
5	B	901	GDP	O6-C6	5.97	1.34	1.23
5	H	901	GDP	O6-C6	5.96	1.34	1.23
5	F	901	GDP	O6-C6	5.96	1.34	1.23
5	L	901	GDP	O6-C6	5.96	1.34	1.23
5	P	901	GDP	O6-C6	5.95	1.34	1.23
5	D	901	GDP	O6-C6	5.92	1.34	1.23
5	P	901	GDP	C8-N9	5.87	1.50	1.37
5	J	901	GDP	C8-N9	5.87	1.50	1.37
5	F	901	GDP	C8-N9	5.87	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	C8-N9	5.87	1.50	1.37
5	B	901	GDP	C8-N9	5.86	1.50	1.37
5	D	901	GDP	C8-N9	5.86	1.50	1.37
5	N	901	GDP	C8-N9	5.86	1.50	1.37
5	R	901	GDP	C8-N9	5.85	1.50	1.37
5	H	901	GDP	C8-N9	5.85	1.50	1.37
3	K	501	GTP	PB-O3A	-5.83	1.53	1.59
3	E	501	GTP	PB-O3A	-5.82	1.53	1.59
3	M	501	GTP	PB-O3A	-5.81	1.53	1.59
3	Q	501	GTP	PB-O3A	-5.81	1.53	1.59
3	O	501	GTP	PB-O3A	-5.80	1.53	1.59
3	G	501	GTP	PB-O3A	-5.79	1.53	1.59
3	I	501	GTP	PB-O3A	-5.77	1.53	1.59
3	A	501	GTP	PB-O3A	-5.76	1.53	1.59
3	C	501	GTP	PB-O3A	-5.70	1.53	1.59
3	K	501	GTP	PB-O3B	5.40	1.65	1.59
3	C	501	GTP	PB-O3B	5.36	1.65	1.59
3	I	501	GTP	PB-O3B	5.36	1.65	1.59
3	M	501	GTP	PB-O3B	5.35	1.65	1.59
3	E	501	GTP	PB-O3B	5.34	1.65	1.59
3	G	501	GTP	PB-O3B	5.34	1.65	1.59
3	A	501	GTP	PB-O3B	5.34	1.65	1.59
3	Q	501	GTP	PB-O3B	5.33	1.65	1.59
3	O	501	GTP	PB-O3B	5.28	1.65	1.59
5	L	901	GDP	C2-N1	4.77	1.49	1.37
5	P	901	GDP	C2-N1	4.75	1.49	1.37
5	J	901	GDP	C2-N1	4.74	1.49	1.37
5	F	901	GDP	C2-N1	4.74	1.49	1.37
5	B	901	GDP	C2-N1	4.73	1.49	1.37
5	D	901	GDP	C2-N1	4.73	1.49	1.37
5	H	901	GDP	C2-N1	4.72	1.49	1.37
5	N	901	GDP	C2-N1	4.72	1.49	1.37
5	R	901	GDP	C2-N1	4.71	1.49	1.37
5	J	901	GDP	PB-O1B	4.35	1.64	1.50
5	B	901	GDP	PB-O1B	4.34	1.64	1.50
5	P	901	GDP	PB-O1B	4.33	1.64	1.50
5	F	901	GDP	PB-O1B	4.33	1.63	1.50
5	D	901	GDP	PB-O1B	4.33	1.63	1.50
5	N	901	GDP	PB-O1B	4.33	1.63	1.50
5	H	901	GDP	PB-O1B	4.32	1.63	1.50
5	R	901	GDP	PB-O1B	4.32	1.63	1.50
5	L	901	GDP	PB-O1B	4.32	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	PB-O2B	-3.92	1.40	1.54
5	D	901	GDP	PB-O2B	-3.92	1.40	1.54
5	R	901	GDP	PB-O2B	-3.91	1.40	1.54
5	B	901	GDP	PB-O2B	-3.91	1.40	1.54
5	P	901	GDP	PB-O2B	-3.91	1.40	1.54
5	J	901	GDP	PB-O2B	-3.91	1.40	1.54
5	N	901	GDP	PB-O2B	-3.91	1.40	1.54
5	H	901	GDP	PB-O2B	-3.90	1.40	1.54
5	F	901	GDP	PB-O2B	-3.90	1.40	1.54
5	R	901	GDP	O4'-C1'	3.40	1.49	1.42
5	D	901	GDP	O4'-C1'	3.39	1.49	1.42
5	J	901	GDP	O4'-C1'	3.39	1.49	1.42
5	H	901	GDP	O4'-C1'	3.39	1.49	1.42
5	B	901	GDP	O4'-C1'	3.39	1.49	1.42
5	F	901	GDP	O4'-C1'	3.39	1.49	1.42
5	N	901	GDP	O4'-C1'	3.38	1.49	1.42
5	P	901	GDP	O4'-C1'	3.38	1.49	1.42
5	L	901	GDP	O4'-C1'	3.37	1.49	1.42
5	L	901	GDP	C8-N7	3.09	1.41	1.32
5	N	901	GDP	C8-N7	3.08	1.41	1.32
5	F	901	GDP	C8-N7	3.08	1.41	1.32
5	J	901	GDP	C8-N7	3.07	1.41	1.32
5	P	901	GDP	C8-N7	3.07	1.41	1.32
5	D	901	GDP	C8-N7	3.07	1.41	1.32
5	B	901	GDP	C8-N7	3.07	1.41	1.32
5	H	901	GDP	C8-N7	3.06	1.41	1.32
5	R	901	GDP	C8-N7	3.06	1.41	1.32
5	P	901	GDP	C5-N7	-2.97	1.33	1.39
5	D	901	GDP	C5-N7	-2.96	1.33	1.39
5	H	901	GDP	C5-N7	-2.94	1.33	1.39
5	N	901	GDP	C5-N7	-2.94	1.33	1.39
5	B	901	GDP	C5-N7	-2.94	1.33	1.39
5	J	901	GDP	C5-N7	-2.94	1.33	1.39
5	L	901	GDP	C5-N7	-2.92	1.33	1.39
5	R	901	GDP	C5-N7	-2.92	1.33	1.39
5	F	901	GDP	C5-N7	-2.91	1.33	1.39
5	J	901	GDP	C5-C4	2.71	1.46	1.38
5	P	901	GDP	C5-C4	2.71	1.46	1.38
5	L	901	GDP	C5-C4	2.70	1.46	1.38
5	H	901	GDP	C5-C4	2.70	1.46	1.38
5	B	901	GDP	C5-C4	2.70	1.46	1.38
5	D	901	GDP	C5-C4	2.69	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	901	GDP	C5-C4	2.68	1.46	1.38
5	N	901	GDP	C5-C4	2.68	1.46	1.38
5	R	901	GDP	C5-C4	2.68	1.46	1.38
5	D	901	GDP	C2-N3	-2.42	1.27	1.33
5	F	901	GDP	C2-N3	-2.42	1.27	1.33
5	N	901	GDP	C2-N3	-2.42	1.27	1.33
5	B	901	GDP	C2-N3	-2.40	1.27	1.33
5	R	901	GDP	C2-N3	-2.40	1.27	1.33
5	L	901	GDP	C2-N3	-2.39	1.27	1.33
5	P	901	GDP	C2-N3	-2.39	1.27	1.33
5	J	901	GDP	C2-N3	-2.39	1.27	1.33
5	H	901	GDP	C2-N3	-2.38	1.27	1.33
5	J	901	GDP	O3'-C3'	2.03	1.48	1.43
5	D	901	GDP	O3'-C3'	2.03	1.48	1.43
5	R	901	GDP	O3'-C3'	2.03	1.48	1.43
5	F	901	GDP	O3'-C3'	2.02	1.48	1.43
5	B	901	GDP	O3'-C3'	2.02	1.47	1.43
5	N	901	GDP	O3'-C3'	2.01	1.47	1.43
5	P	901	GDP	O3'-C3'	2.01	1.47	1.43
5	L	901	GDP	O3'-C3'	2.00	1.47	1.43

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GDP	N9-C8-N7	-10.79	93.39	113.40
5	L	901	GDP	N9-C8-N7	-10.79	93.39	113.40
5	F	901	GDP	N9-C8-N7	-10.79	93.39	113.40
5	P	901	GDP	N9-C8-N7	-10.78	93.40	113.40
5	N	901	GDP	N9-C8-N7	-10.78	93.40	113.40
5	B	901	GDP	N9-C8-N7	-10.78	93.41	113.40
5	D	901	GDP	N9-C8-N7	-10.77	93.42	113.40
5	R	901	GDP	N9-C8-N7	-10.77	93.42	113.40
5	H	901	GDP	N9-C8-N7	-10.76	93.44	113.40
5	P	901	GDP	C8-N7-C5	9.29	120.80	104.26
5	J	901	GDP	C8-N7-C5	9.28	120.79	104.26
5	B	901	GDP	C8-N7-C5	9.27	120.78	104.26
5	D	901	GDP	C8-N7-C5	9.27	120.77	104.26
5	R	901	GDP	C8-N7-C5	9.26	120.76	104.26
5	H	901	GDP	C8-N7-C5	9.26	120.75	104.26
5	N	901	GDP	C8-N7-C5	9.26	120.75	104.26
5	L	901	GDP	C8-N7-C5	9.25	120.73	104.26
5	F	901	GDP	C8-N7-C5	9.24	120.72	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GDP	C6-C5-N7	8.70	146.12	130.29
5	P	901	GDP	C6-C5-N7	8.66	146.06	130.29
5	B	901	GDP	C6-C5-N7	8.66	146.04	130.29
5	H	901	GDP	C6-C5-N7	8.64	146.02	130.29
5	R	901	GDP	C6-C5-N7	8.64	146.02	130.29
5	D	901	GDP	C6-C5-N7	8.64	146.01	130.29
5	N	901	GDP	C6-C5-N7	8.64	146.01	130.29
5	L	901	GDP	C6-C5-N7	8.62	145.99	130.29
5	F	901	GDP	C6-C5-N7	8.62	145.98	130.29
5	J	901	GDP	C6-C5-C4	-6.29	109.37	118.83
5	L	901	GDP	N2-C2-N3	6.28	131.93	119.67
5	D	901	GDP	N2-C2-N3	6.27	131.91	119.67
5	P	901	GDP	C6-C5-C4	-6.26	109.42	118.83
5	N	901	GDP	N2-C2-N3	6.26	131.88	119.67
5	N	901	GDP	C6-C5-C4	-6.26	109.42	118.83
5	B	901	GDP	N2-C2-N3	6.25	131.88	119.67
5	B	901	GDP	C6-C5-C4	-6.25	109.42	118.83
5	P	901	GDP	N2-C2-N3	6.25	131.87	119.67
5	L	901	GDP	C6-C5-C4	-6.25	109.43	118.83
5	R	901	GDP	N2-C2-N3	6.25	131.87	119.67
5	D	901	GDP	C6-C5-C4	-6.24	109.44	118.83
5	H	901	GDP	C6-C5-C4	-6.24	109.44	118.83
5	H	901	GDP	N2-C2-N3	6.24	131.84	119.67
5	J	901	GDP	N2-C2-N3	6.23	131.84	119.67
5	F	901	GDP	C6-C5-C4	-6.23	109.45	118.83
5	R	901	GDP	C6-C5-C4	-6.23	109.45	118.83
5	F	901	GDP	N2-C2-N3	6.23	131.83	119.67
5	L	901	GDP	C8-N9-C4	5.90	117.09	106.03
5	F	901	GDP	C8-N9-C4	5.89	117.07	106.03
5	J	901	GDP	C8-N9-C4	5.88	117.06	106.03
5	N	901	GDP	C8-N9-C4	5.87	117.04	106.03
5	B	901	GDP	C8-N9-C4	5.87	117.03	106.03
5	H	901	GDP	C8-N9-C4	5.86	117.02	106.03
5	P	901	GDP	C8-N9-C4	5.86	117.01	106.03
5	R	901	GDP	C8-N9-C4	5.86	117.01	106.03
5	D	901	GDP	C8-N9-C4	5.86	117.00	106.03
5	J	901	GDP	C5-C6-N1	4.54	124.80	113.25
5	P	901	GDP	C5-C6-N1	4.52	124.76	113.25
5	B	901	GDP	C5-C6-N1	4.51	124.73	113.25
5	H	901	GDP	C5-C6-N1	4.50	124.71	113.25
5	R	901	GDP	C5-C6-N1	4.50	124.71	113.25
5	L	901	GDP	C5-C6-N1	4.50	124.71	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	901	GDP	C5-C6-N1	4.50	124.71	113.25
5	N	901	GDP	C5-C6-N1	4.50	124.69	113.25
5	D	901	GDP	C5-C6-N1	4.48	124.67	113.25
5	D	901	GDP	N2-C2-N1	-4.23	107.84	116.76
5	N	901	GDP	N2-C2-N1	-4.22	107.86	116.76
5	L	901	GDP	N2-C2-N1	-4.22	107.86	116.76
5	P	901	GDP	N2-C2-N1	-4.22	107.86	116.76
5	B	901	GDP	N2-C2-N1	-4.21	107.88	116.76
5	R	901	GDP	N2-C2-N1	-4.20	107.89	116.76
5	F	901	GDP	N2-C2-N1	-4.19	107.91	116.76
5	H	901	GDP	N2-C2-N1	-4.19	107.92	116.76
5	J	901	GDP	N2-C2-N1	-4.19	107.92	116.76
5	L	901	GDP	C2-N3-C4	4.08	119.32	112.30
5	F	901	GDP	C2-N3-C4	4.06	119.30	112.30
5	R	901	GDP	C2-N3-C4	4.06	119.29	112.30
5	D	901	GDP	C2-N3-C4	4.06	119.28	112.30
5	B	901	GDP	C2-N3-C4	4.05	119.28	112.30
5	H	901	GDP	C2-N3-C4	4.05	119.28	112.30
5	J	901	GDP	C2-N3-C4	4.05	119.28	112.30
5	N	901	GDP	C2-N3-C4	4.05	119.28	112.30
5	P	901	GDP	C2-N3-C4	4.03	119.24	112.30
5	J	901	GDP	O6-C6-C5	-4.02	115.92	126.53
5	N	901	GDP	O6-C6-C5	-4.00	115.97	126.53
5	B	901	GDP	O6-C6-C5	-3.99	115.99	126.53
5	R	901	GDP	O6-C6-C5	-3.99	115.99	126.53
5	H	901	GDP	O6-C6-C5	-3.99	115.99	126.53
5	F	901	GDP	O6-C6-C5	-3.99	116.01	126.53
5	P	901	GDP	O6-C6-C5	-3.99	116.01	126.53
5	D	901	GDP	O6-C6-C5	-3.98	116.01	126.53
5	L	901	GDP	O6-C6-C5	-3.98	116.03	126.53
5	J	901	GDP	C4-C5-N7	-3.89	104.51	110.67
5	R	901	GDP	C4-C5-N7	-3.88	104.52	110.67
5	P	901	GDP	C4-C5-N7	-3.88	104.53	110.67
5	B	901	GDP	C4-C5-N7	-3.88	104.53	110.67
5	H	901	GDP	C4-C5-N7	-3.87	104.53	110.67
5	D	901	GDP	C4-C5-N7	-3.86	104.55	110.67
5	N	901	GDP	C4-C5-N7	-3.85	104.57	110.67
5	F	901	GDP	C4-C5-N7	-3.85	104.57	110.67
5	L	901	GDP	C4-C5-N7	-3.84	104.58	110.67
5	P	901	GDP	C2-N1-C6	-3.76	118.29	125.11
5	J	901	GDP	C2-N1-C6	-3.75	118.32	125.11
5	B	901	GDP	C2-N1-C6	-3.74	118.33	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	901	GDP	C2-N1-C6	-3.74	118.33	125.11
5	L	901	GDP	C2-N1-C6	-3.74	118.33	125.11
5	N	901	GDP	C2-N1-C6	-3.74	118.33	125.11
5	R	901	GDP	C2-N1-C6	-3.74	118.34	125.11
5	H	901	GDP	C2-N1-C6	-3.73	118.35	125.11
5	D	901	GDP	C2-N1-C6	-3.72	118.36	125.11
5	J	901	GDP	C2'-C3'-C4'	3.48	109.34	102.61
5	L	901	GDP	C2'-C3'-C4'	3.48	109.33	102.61
5	F	901	GDP	C2'-C3'-C4'	3.48	109.32	102.61
5	P	901	GDP	C2'-C3'-C4'	3.47	109.31	102.61
5	B	901	GDP	C2'-C3'-C4'	3.46	109.30	102.61
5	H	901	GDP	C2'-C3'-C4'	3.46	109.29	102.61
5	D	901	GDP	C2'-C3'-C4'	3.45	109.28	102.61
5	N	901	GDP	C2'-C3'-C4'	3.45	109.28	102.61
5	R	901	GDP	C2'-C3'-C4'	3.44	109.26	102.61
5	J	901	GDP	C1'-N9-C8	-2.68	119.11	126.73
5	P	901	GDP	C1'-N9-C8	-2.67	119.14	126.73
5	L	901	GDP	C1'-N9-C8	-2.67	119.15	126.73
5	F	901	GDP	C1'-N9-C8	-2.66	119.16	126.73
5	D	901	GDP	C1'-N9-C8	-2.66	119.17	126.73
3	G	501	GTP	O2G-PG-O3B	2.66	113.56	104.64
5	B	901	GDP	C1'-N9-C8	-2.66	119.17	126.73
5	N	901	GDP	C1'-N9-C8	-2.66	119.17	126.73
5	R	901	GDP	C1'-N9-C8	-2.66	119.18	126.73
3	Q	501	GTP	O2G-PG-O3B	2.66	113.55	104.64
3	E	501	GTP	O2G-PG-O3B	2.66	113.54	104.64
3	M	501	GTP	O2G-PG-O3B	2.65	113.52	104.64
3	K	501	GTP	O2G-PG-O3B	2.65	113.52	104.64
3	A	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
3	C	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
5	H	901	GDP	C1'-N9-C8	-2.64	119.23	126.73
3	I	501	GTP	O2G-PG-O3B	2.64	113.48	104.64
3	O	501	GTP	O2G-PG-O3B	2.63	113.47	104.64
5	P	901	GDP	O2'-C2'-C3'	2.34	119.31	111.82
5	F	901	GDP	O2'-C2'-C3'	2.33	119.30	111.82
5	J	901	GDP	O2'-C2'-C3'	2.33	119.29	111.82
5	H	901	GDP	O2'-C2'-C3'	2.33	119.29	111.82
5	B	901	GDP	O2'-C2'-C3'	2.33	119.28	111.82
5	N	901	GDP	O2'-C2'-C3'	2.33	119.27	111.82
5	R	901	GDP	O2'-C2'-C3'	2.32	119.26	111.82
5	D	901	GDP	O2'-C2'-C3'	2.32	119.26	111.82
5	L	901	GDP	O2'-C2'-C3'	2.32	119.25	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	901	GDP	O3B-PB-O2B	2.22	116.12	107.80
5	J	901	GDP	O3B-PB-O2B	2.21	116.10	107.80
5	D	901	GDP	O3B-PB-O2B	2.21	116.10	107.80
5	F	901	GDP	O3B-PB-O2B	2.21	116.09	107.80
5	P	901	GDP	O3B-PB-O2B	2.21	116.09	107.80
5	L	901	GDP	O3B-PB-O2B	2.21	116.09	107.80
5	B	901	GDP	O3B-PB-O2B	2.21	116.09	107.80
5	R	901	GDP	O3B-PB-O2B	2.21	116.08	107.80
5	H	901	GDP	O3B-PB-O2B	2.20	116.07	107.80
3	G	501	GTP	O5'-C5'-C4'	2.10	116.16	108.99
3	Q	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
5	F	901	GDP	C4'-O4'-C1'	2.10	114.10	109.47
3	C	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
3	I	501	GTP	O5'-C5'-C4'	2.10	116.13	108.99
3	A	501	GTP	O5'-C5'-C4'	2.10	116.13	108.99
3	E	501	GTP	O5'-C5'-C4'	2.09	116.12	108.99
3	O	501	GTP	O5'-C5'-C4'	2.09	116.12	108.99
5	H	901	GDP	C4'-O4'-C1'	2.09	114.08	109.47
3	M	501	GTP	O5'-C5'-C4'	2.09	116.10	108.99
5	L	901	GDP	C4'-O4'-C1'	2.08	114.07	109.47
3	K	501	GTP	O5'-C5'-C4'	2.08	116.09	108.99
5	P	901	GDP	C4'-O4'-C1'	2.08	114.05	109.47
5	N	901	GDP	C4'-O4'-C1'	2.07	114.04	109.47
5	B	901	GDP	C4'-O4'-C1'	2.07	114.04	109.47
5	J	901	GDP	C4'-O4'-C1'	2.07	114.03	109.47
5	D	901	GDP	C4'-O4'-C1'	2.05	114.00	109.47
3	M	501	GTP	O3G-PG-O3B	2.05	111.51	104.64
3	G	501	GTP	O3G-PG-O3B	2.05	111.50	104.64
5	R	901	GDP	C4'-O4'-C1'	2.05	113.98	109.47
3	A	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
3	E	501	GTP	O3G-PG-O3B	2.04	111.49	104.64
3	I	501	GTP	O3G-PG-O3B	2.04	111.48	104.64
3	C	501	GTP	O3G-PG-O3B	2.04	111.48	104.64
3	K	501	GTP	O3G-PG-O3B	2.04	111.47	104.64
3	O	501	GTP	O3G-PG-O3B	2.04	111.46	104.64
3	Q	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
5	L	901	GDP	O4'-C4'-C3'	-2.00	101.17	105.15
5	F	901	GDP	O4'-C4'-C3'	-2.00	101.18	105.15

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	GDP	PA-O3A-PB-O2B
5	B	901	GDP	C5'-O5'-PA-O3A
5	B	901	GDP	C5'-O5'-PA-O2A
5	D	901	GDP	PA-O3A-PB-O2B
5	D	901	GDP	C5'-O5'-PA-O3A
5	D	901	GDP	C5'-O5'-PA-O2A
5	F	901	GDP	PA-O3A-PB-O2B
5	F	901	GDP	C5'-O5'-PA-O3A
5	F	901	GDP	C5'-O5'-PA-O2A
5	H	901	GDP	PA-O3A-PB-O2B
5	H	901	GDP	C5'-O5'-PA-O3A
5	H	901	GDP	C5'-O5'-PA-O2A
5	J	901	GDP	PA-O3A-PB-O2B
5	J	901	GDP	C5'-O5'-PA-O3A
5	J	901	GDP	C5'-O5'-PA-O2A
5	L	901	GDP	PA-O3A-PB-O2B
5	L	901	GDP	C5'-O5'-PA-O3A
5	L	901	GDP	C5'-O5'-PA-O2A
5	N	901	GDP	PA-O3A-PB-O2B
5	N	901	GDP	C5'-O5'-PA-O3A
5	N	901	GDP	C5'-O5'-PA-O2A
5	P	901	GDP	PA-O3A-PB-O2B
5	P	901	GDP	C5'-O5'-PA-O3A
5	P	901	GDP	C5'-O5'-PA-O2A
5	R	901	GDP	PA-O3A-PB-O2B
5	R	901	GDP	C5'-O5'-PA-O3A
5	R	901	GDP	C5'-O5'-PA-O2A
3	A	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	Q	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	A	501	GTP	O4'-C4'-C5'-O5'
3	I	501	GTP	O4'-C4'-C5'-O5'
3	K	501	GTP	O4'-C4'-C5'-O5'
3	M	501	GTP	O4'-C4'-C5'-O5'
3	O	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	E	501	GTP	C5'-O5'-PA-O1A
3	G	501	GTP	C5'-O5'-PA-O1A
3	I	501	GTP	C5'-O5'-PA-O1A
3	K	501	GTP	C5'-O5'-PA-O1A
3	M	501	GTP	C5'-O5'-PA-O1A
3	O	501	GTP	C5'-O5'-PA-O1A
3	Q	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	O4'-C4'-C5'-O5'
3	E	501	GTP	O4'-C4'-C5'-O5'
3	G	501	GTP	O4'-C4'-C5'-O5'
3	Q	501	GTP	O4'-C4'-C5'-O5'
5	B	901	GDP	PA-O3A-PB-O3B
5	D	901	GDP	PA-O3A-PB-O3B
5	F	901	GDP	PA-O3A-PB-O3B
5	H	901	GDP	PA-O3A-PB-O3B
5	J	901	GDP	PA-O3A-PB-O3B
5	L	901	GDP	PA-O3A-PB-O3B
5	N	901	GDP	PA-O3A-PB-O3B
5	P	901	GDP	PA-O3A-PB-O3B
5	R	901	GDP	PA-O3A-PB-O3B
3	A	501	GTP	PG-O3B-PB-O2B
3	C	501	GTP	PG-O3B-PB-O2B
3	E	501	GTP	PG-O3B-PB-O2B
3	G	501	GTP	PG-O3B-PB-O2B
3	I	501	GTP	PG-O3B-PB-O2B
3	K	501	GTP	PG-O3B-PB-O2B
3	M	501	GTP	PG-O3B-PB-O2B
3	O	501	GTP	PG-O3B-PB-O2B
3	Q	501	GTP	PG-O3B-PB-O2B

There are no ring outliers.

18 monomers are involved in 36 short contacts:

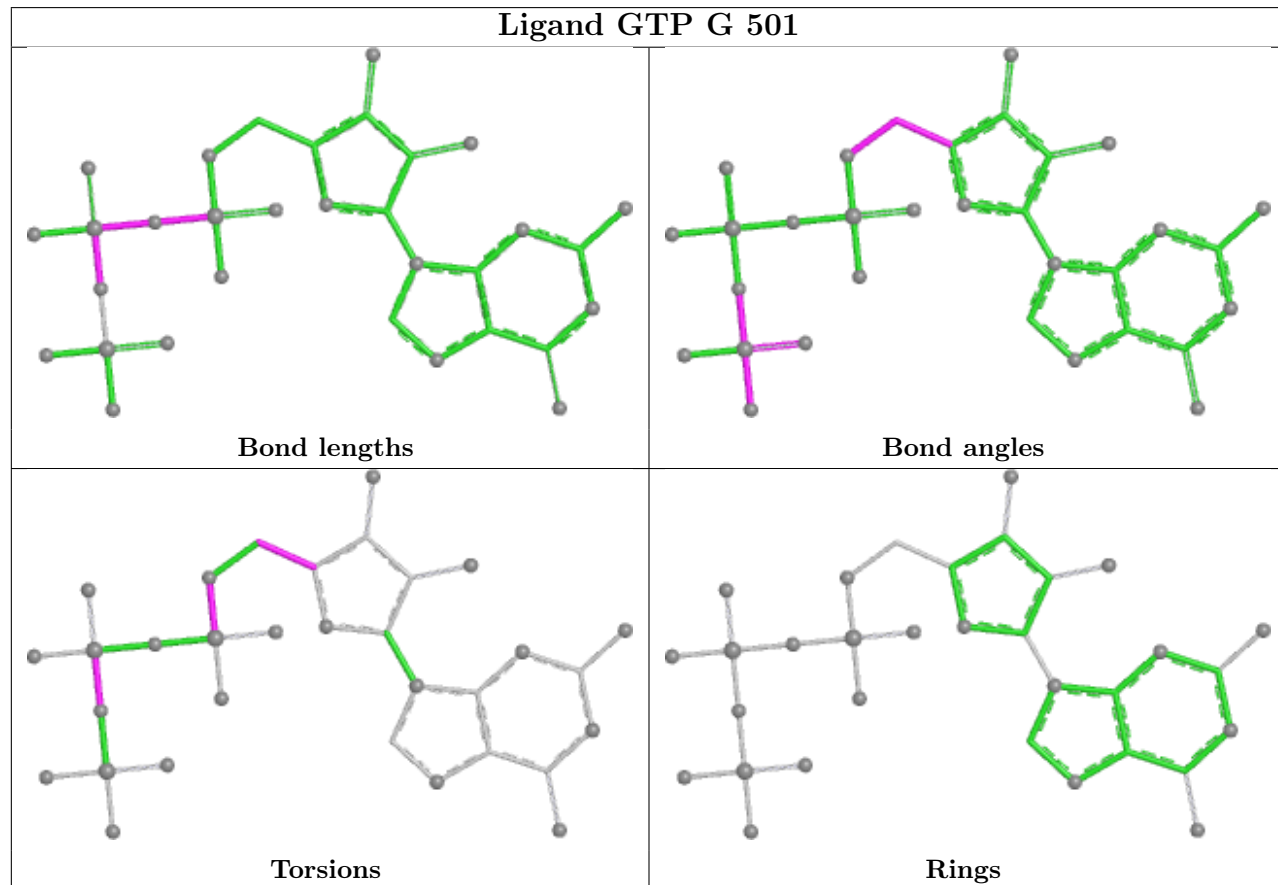
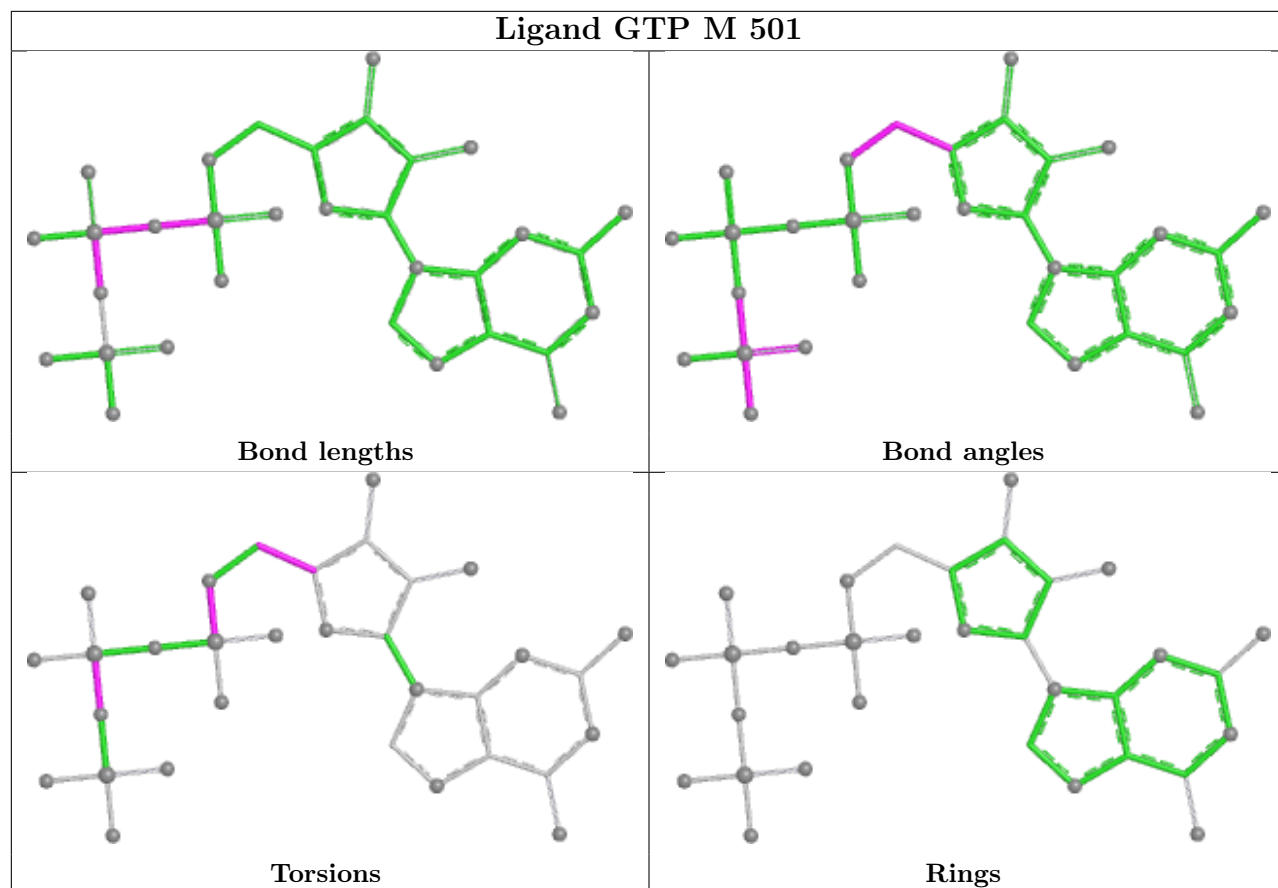
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	501	GTP	2	0
3	G	501	GTP	2	0
3	Q	501	GTP	2	0
5	D	901	GDP	2	0
5	L	901	GDP	2	0
5	H	901	GDP	2	0
3	O	501	GTP	2	0
3	A	501	GTP	2	0

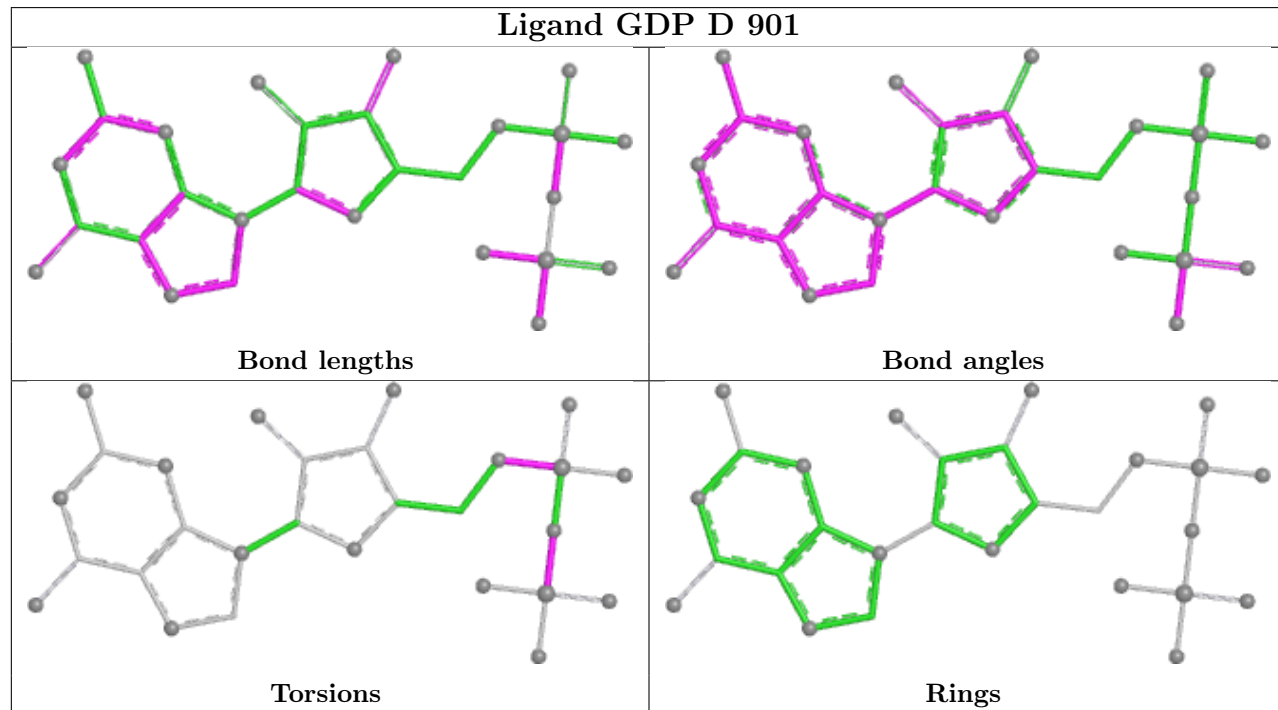
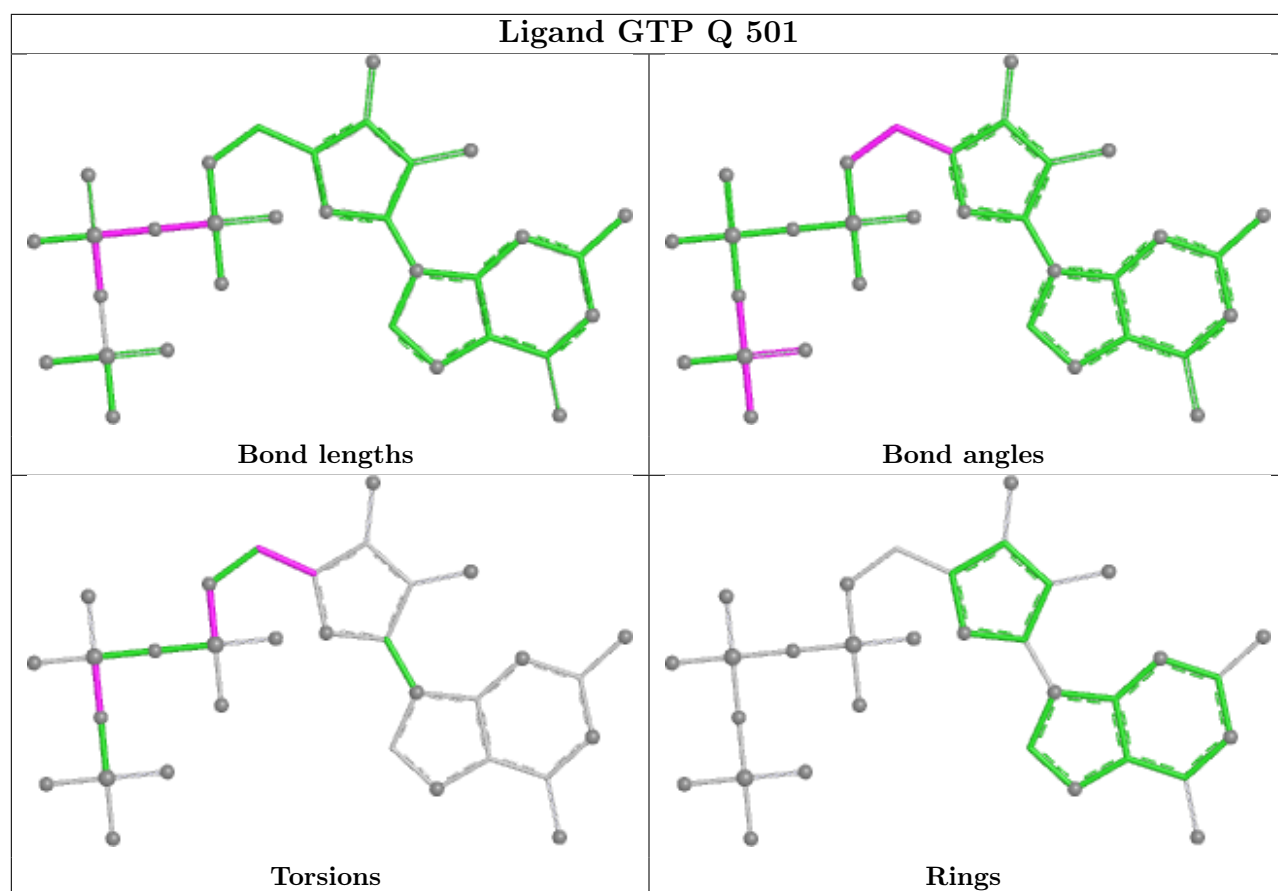
Continued on next page...

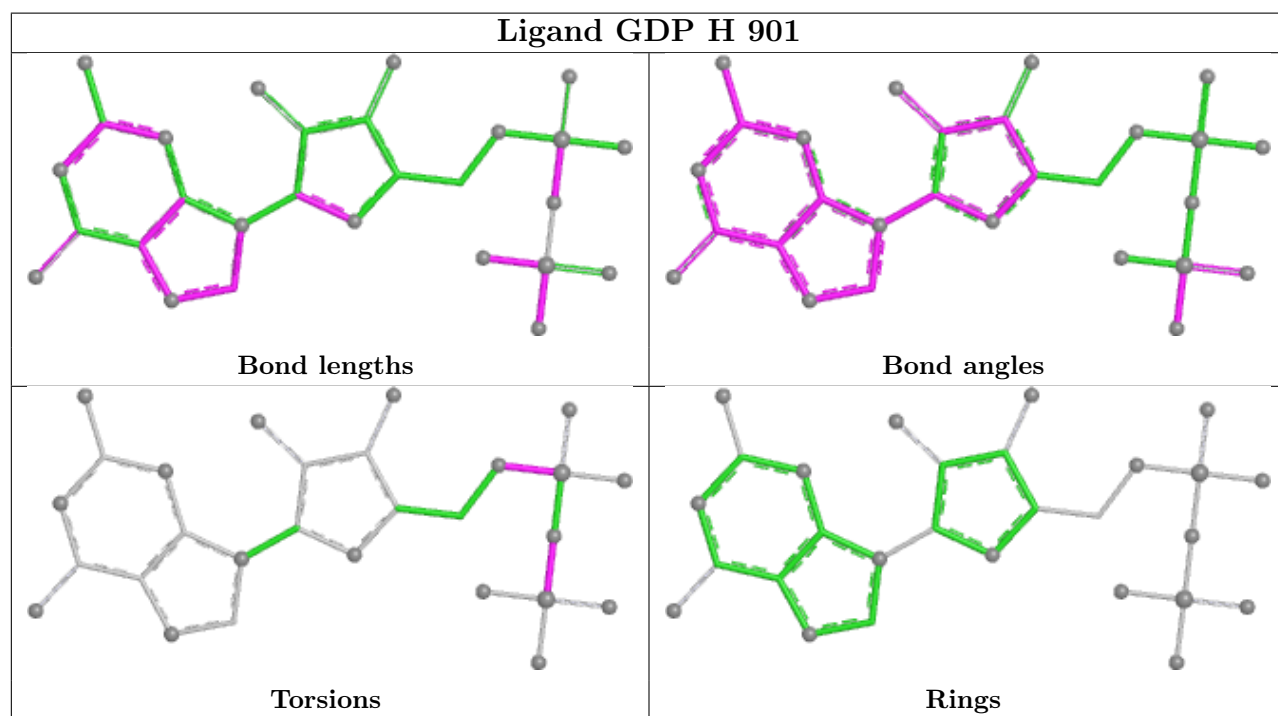
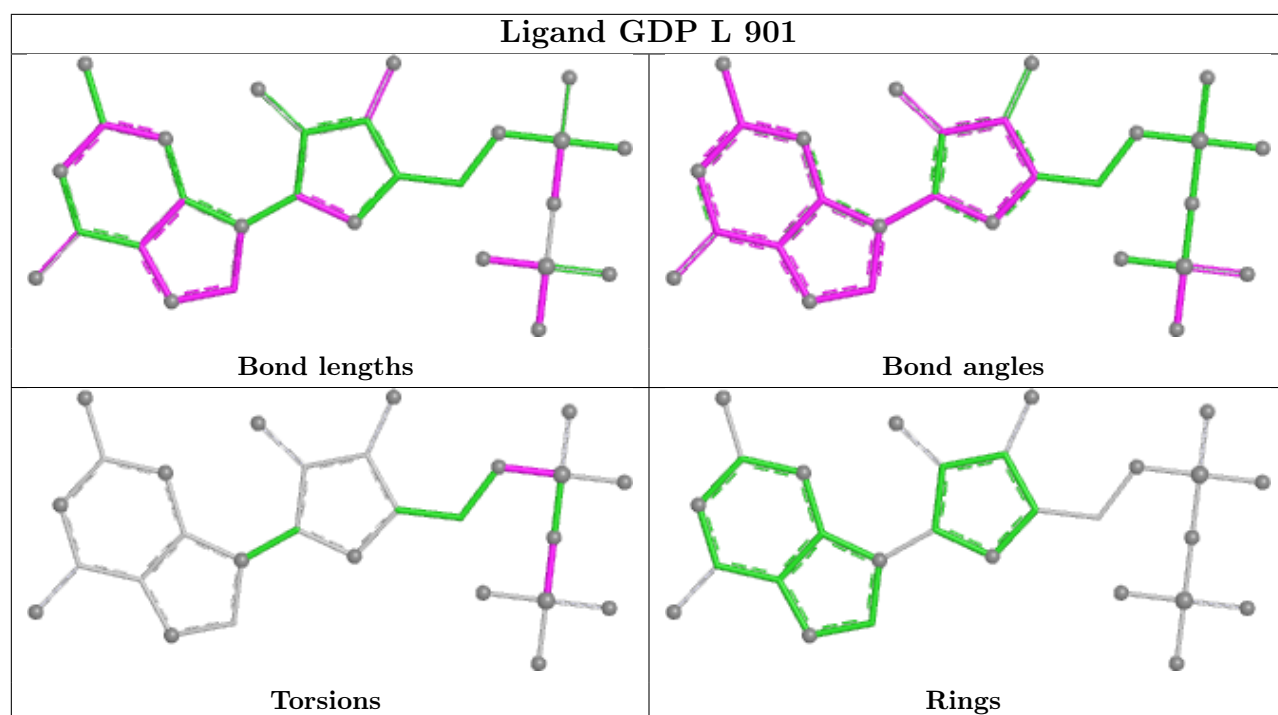
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	GTP	2	0
5	B	901	GDP	2	0
3	K	501	GTP	2	0
3	I	501	GTP	2	0
5	J	901	GDP	2	0
5	N	901	GDP	2	0
5	P	901	GDP	2	0
3	C	501	GTP	2	0
5	F	901	GDP	2	0
5	R	901	GDP	2	0

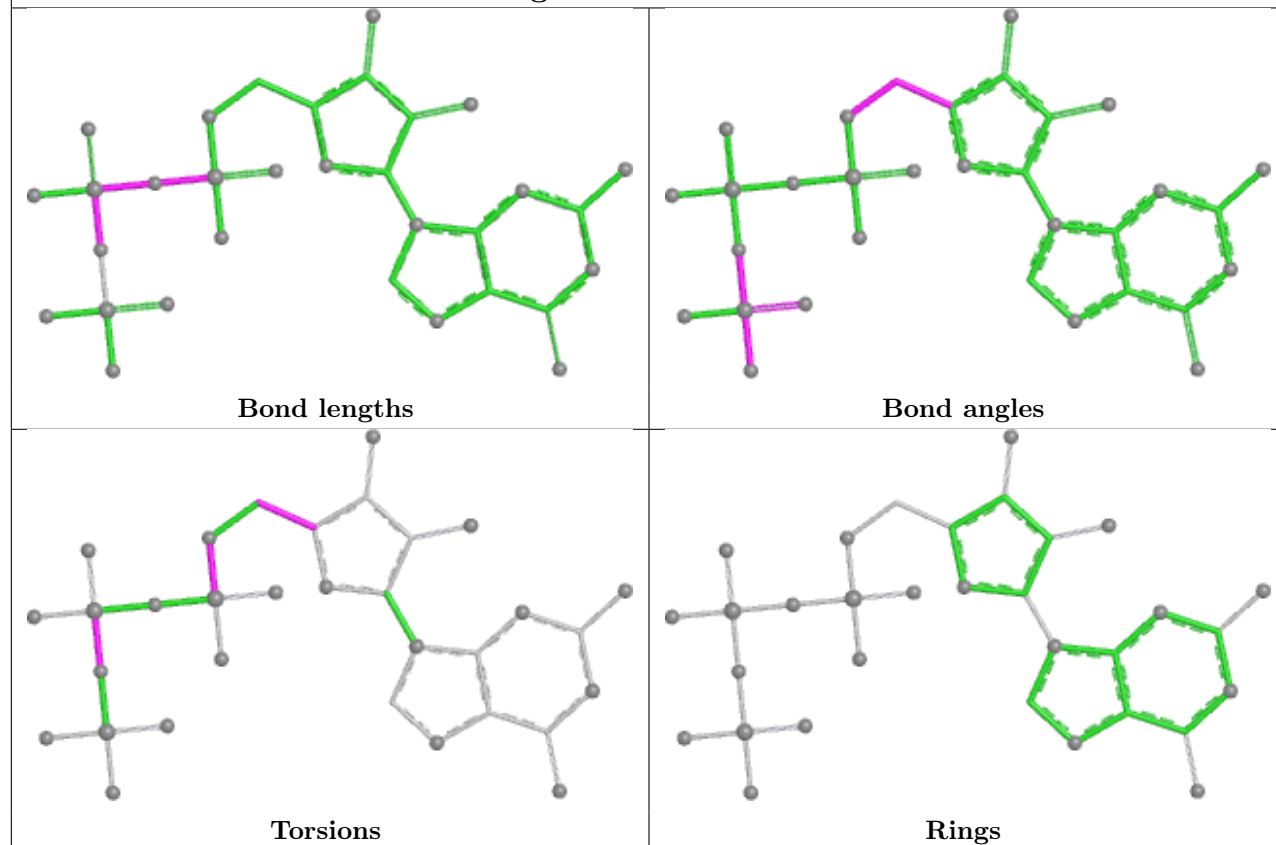
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



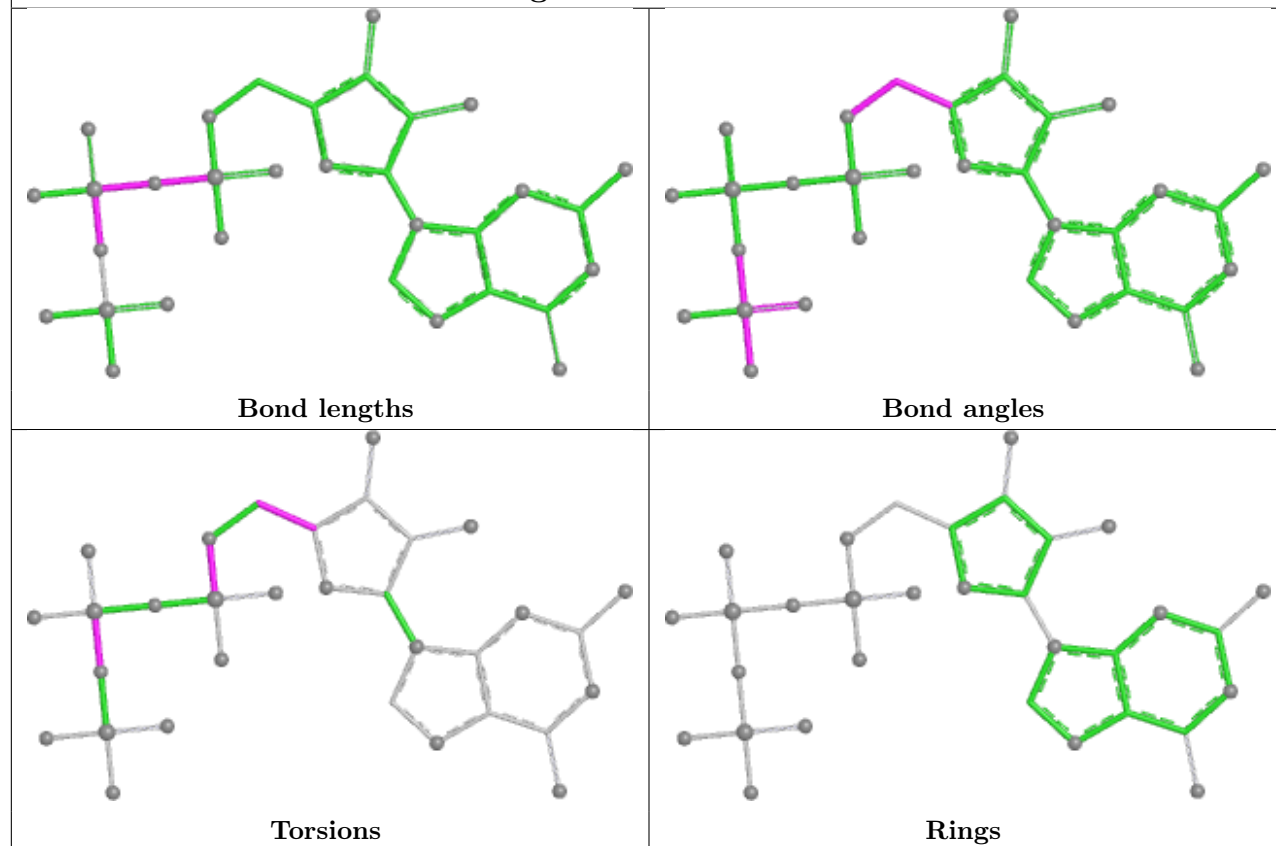




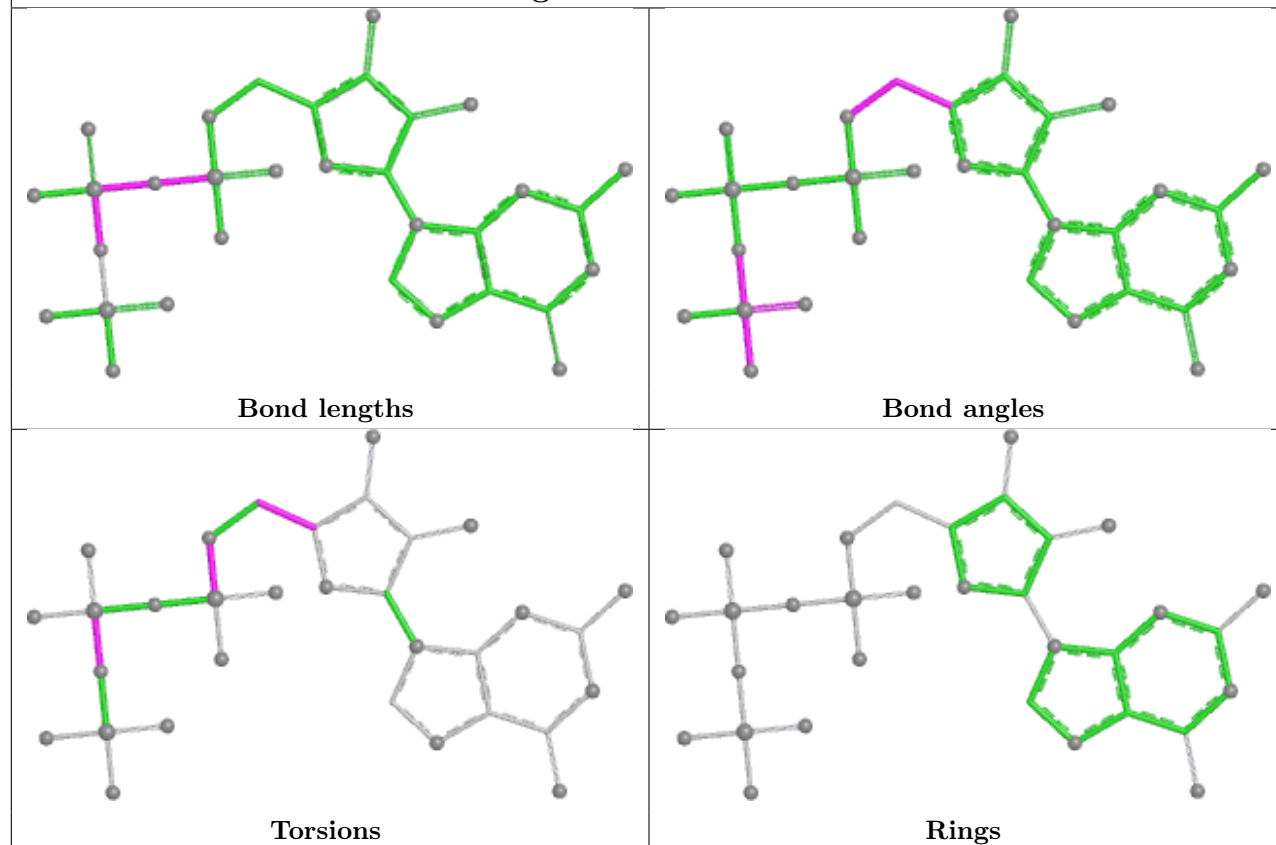
Ligand GTP O 501



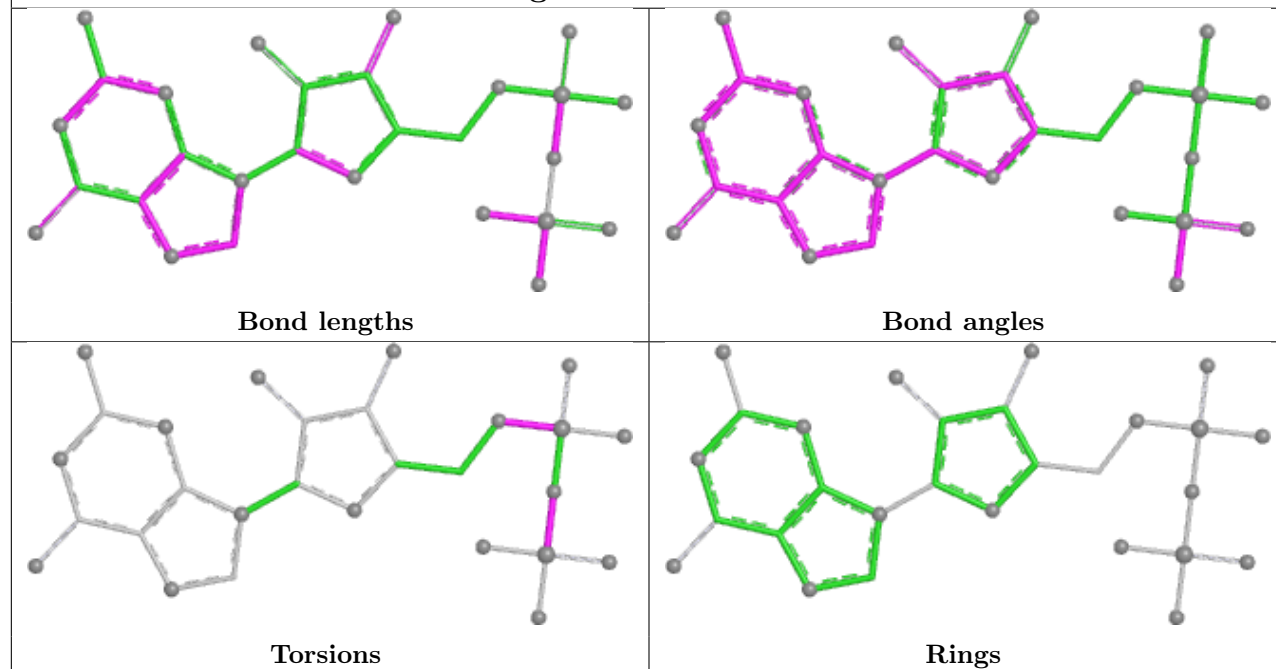
Ligand GTP A 501

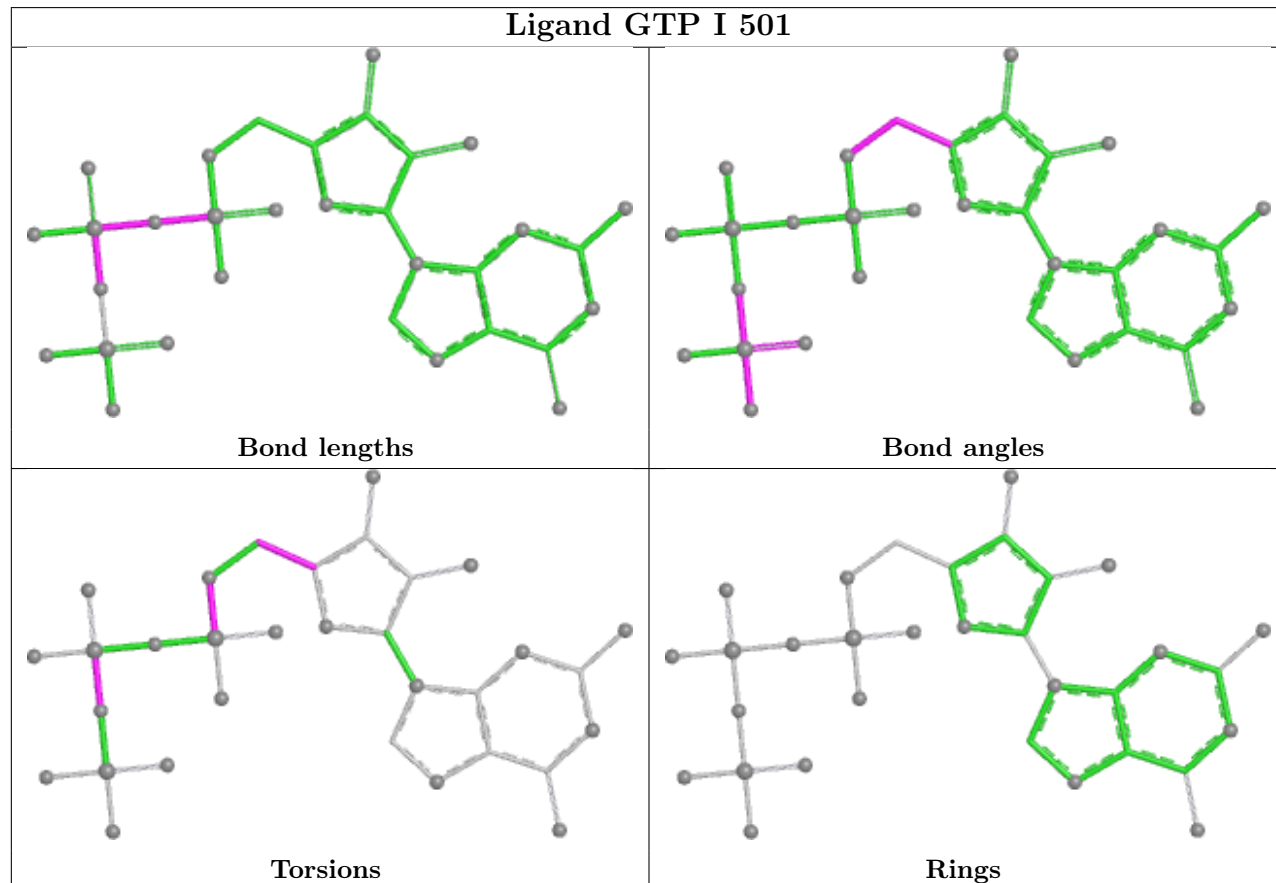
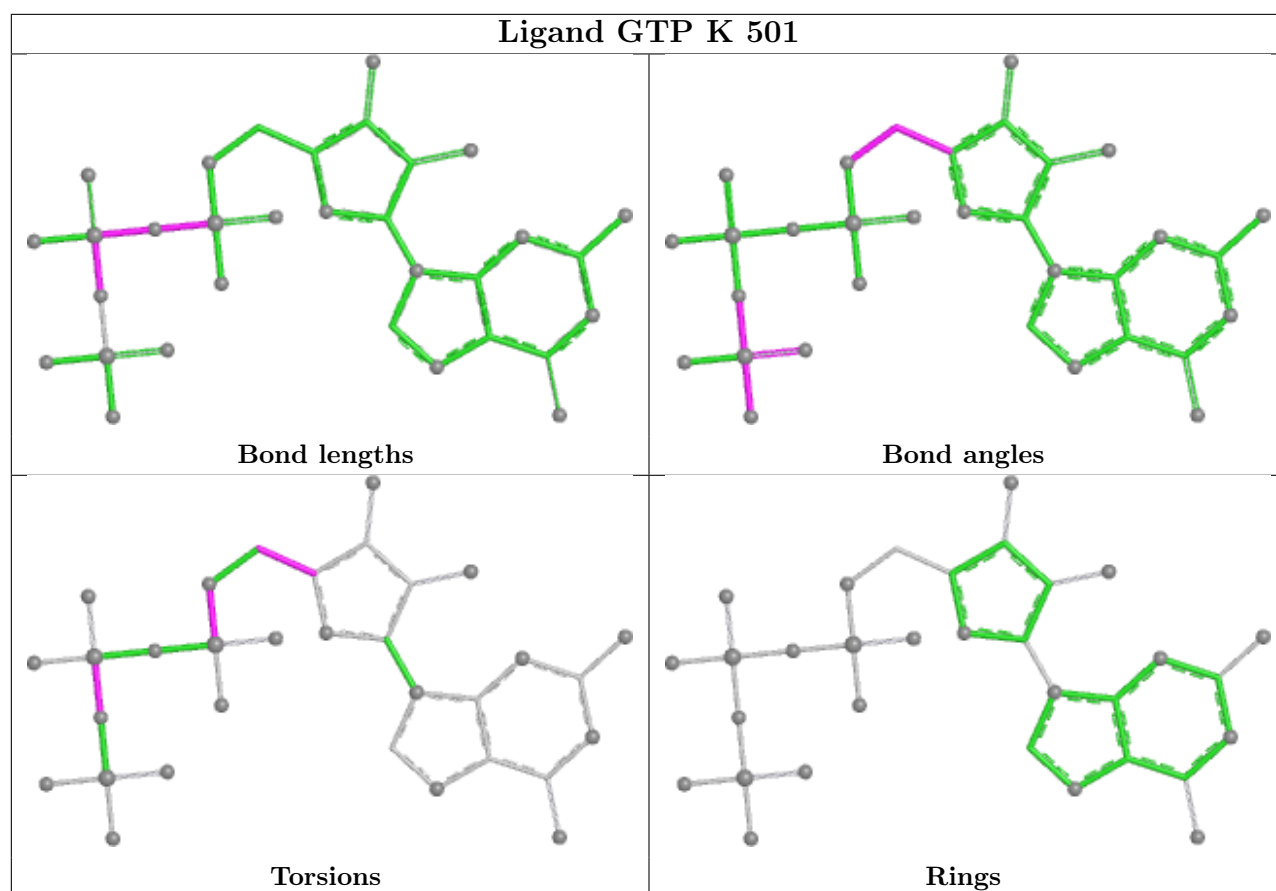


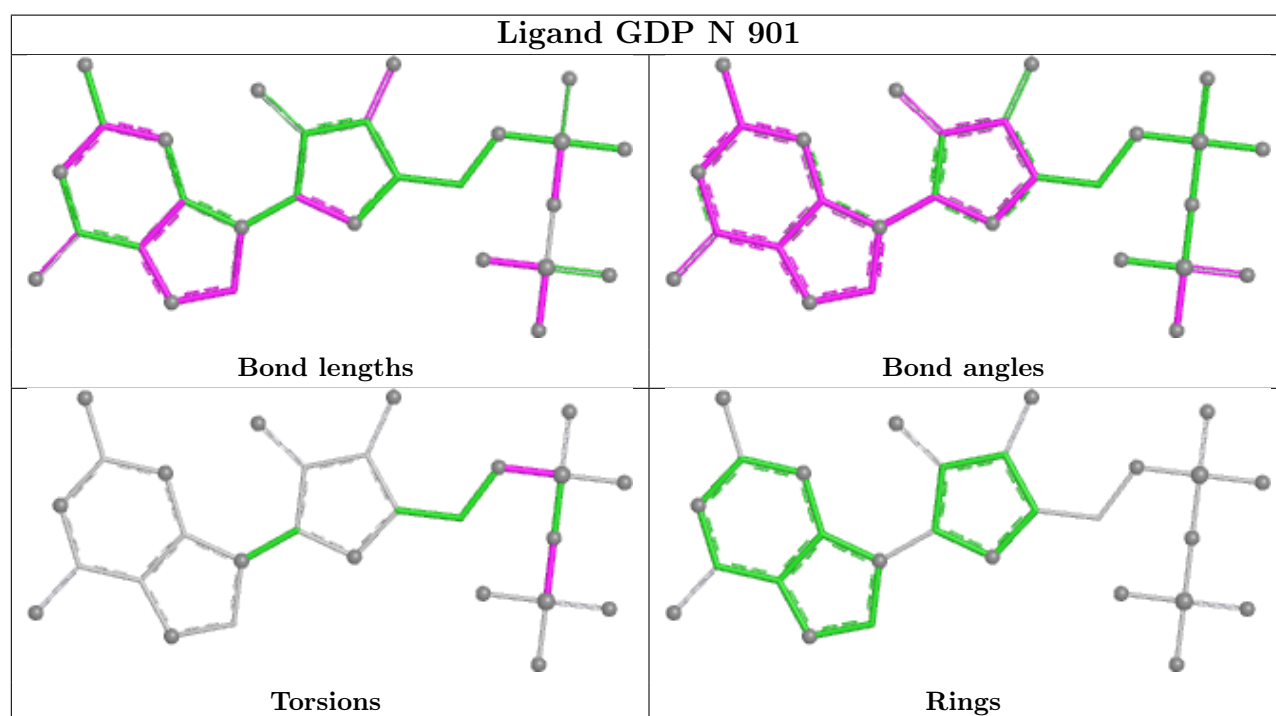
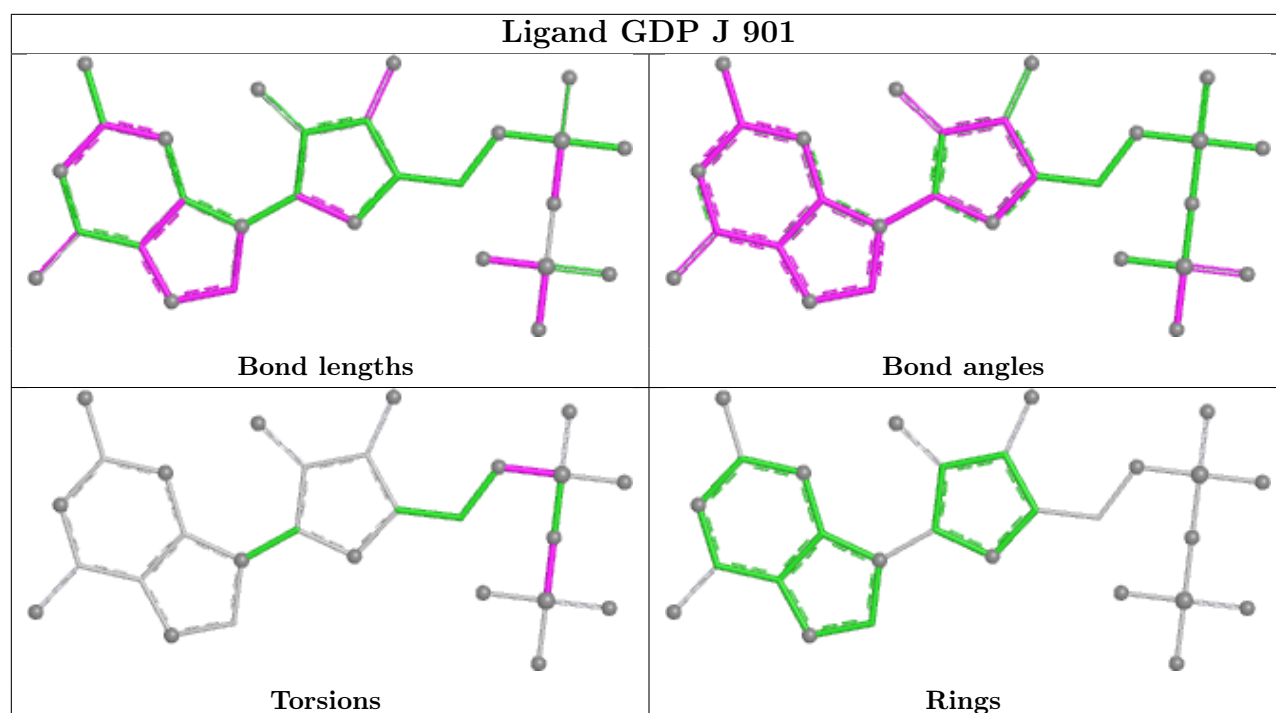
Ligand GTP E 501

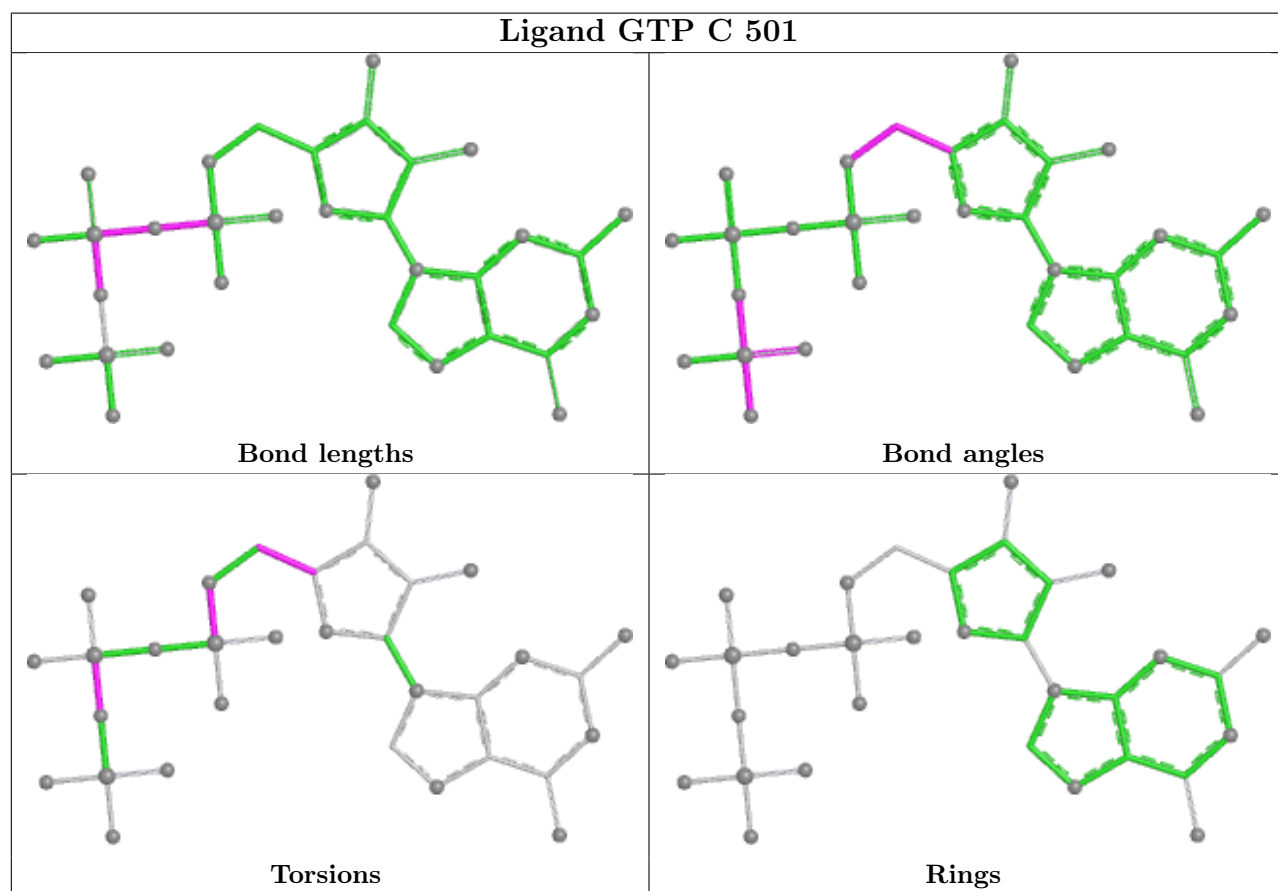
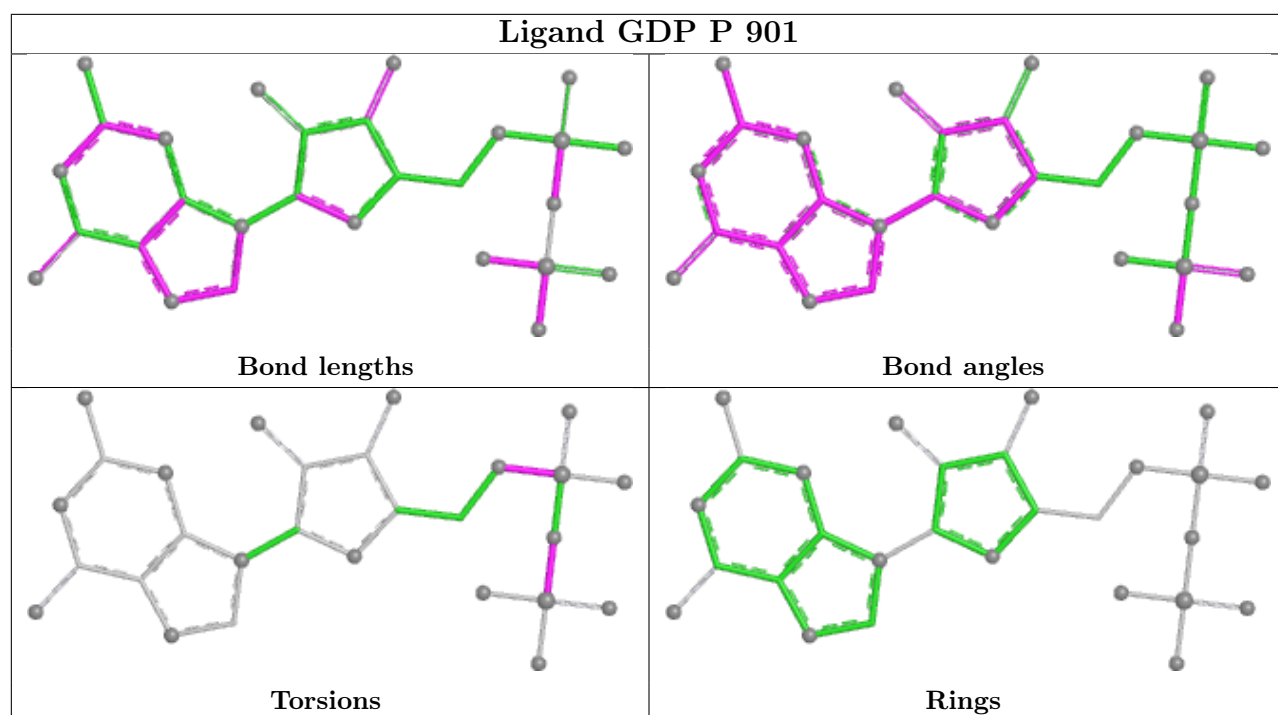


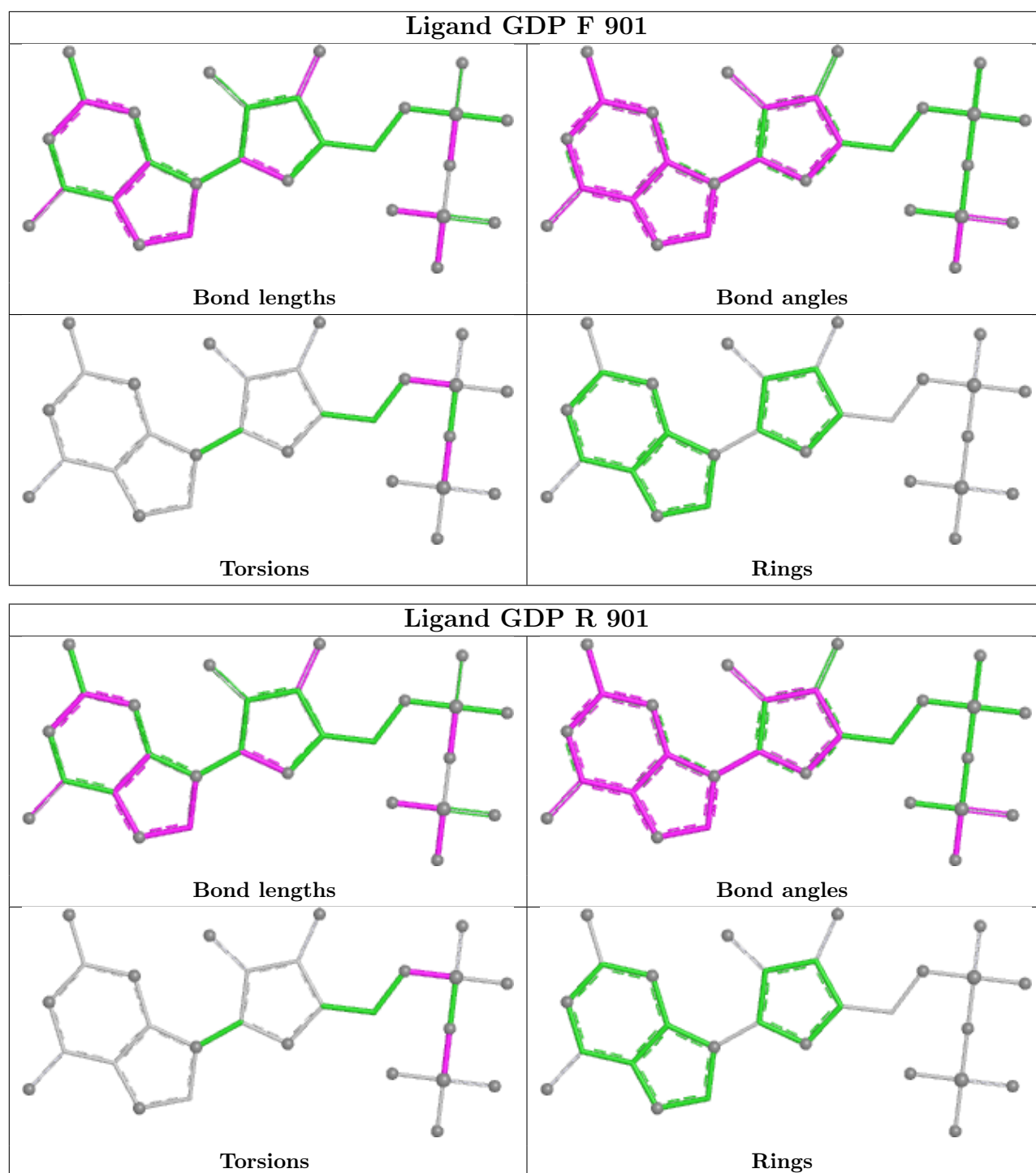
Ligand GDP B 901











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

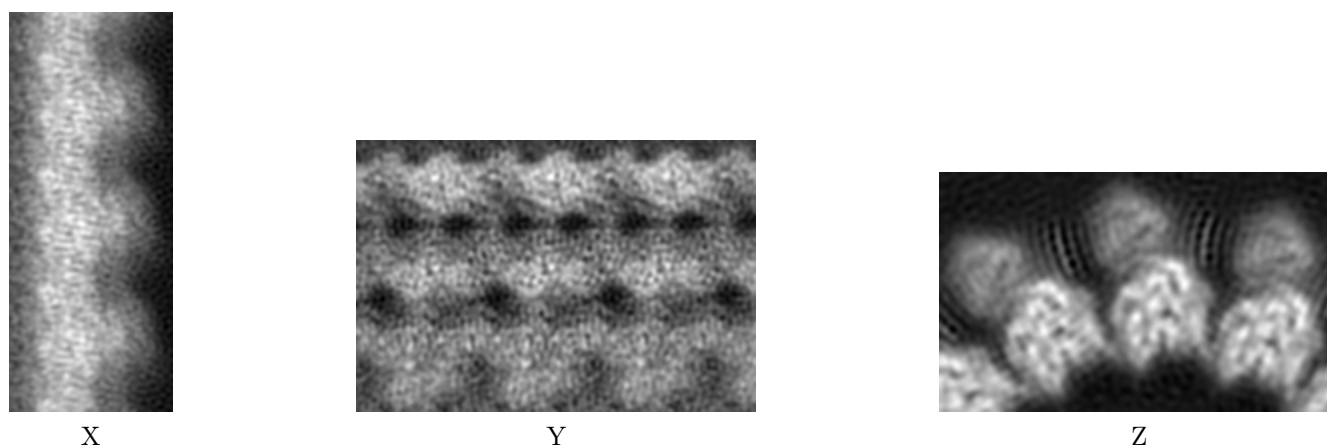
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5896. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

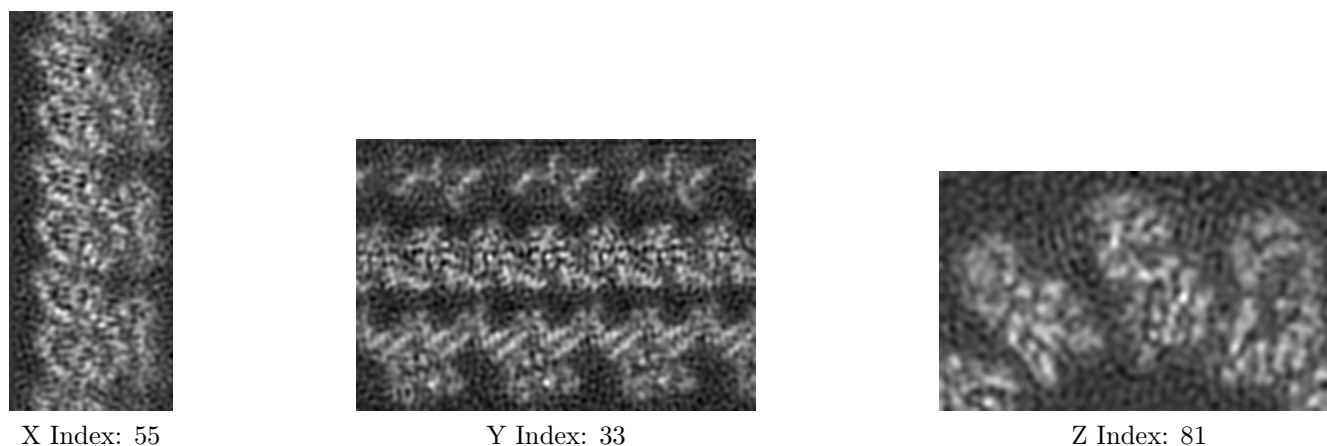
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

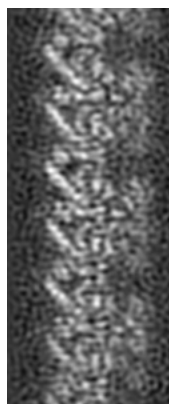
6.2.1 Primary map



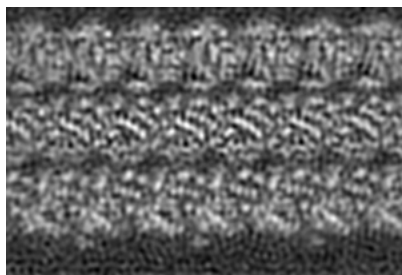
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

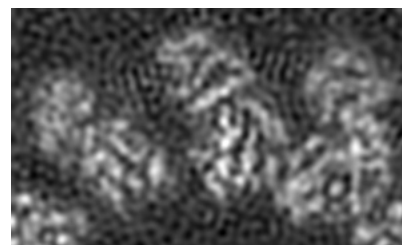
6.3.1 Primary map



X Index: 59



Y Index: 23

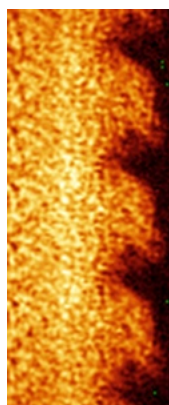


Z Index: 79

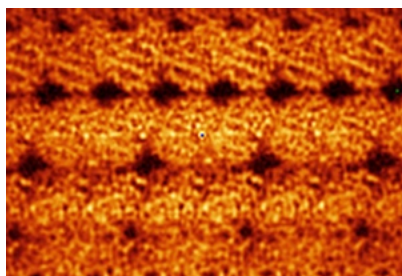
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

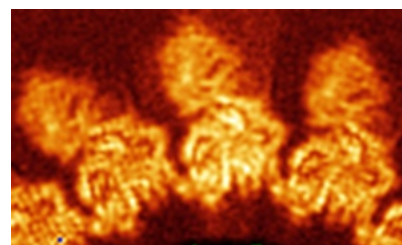
6.4.1 Primary map



X



Y

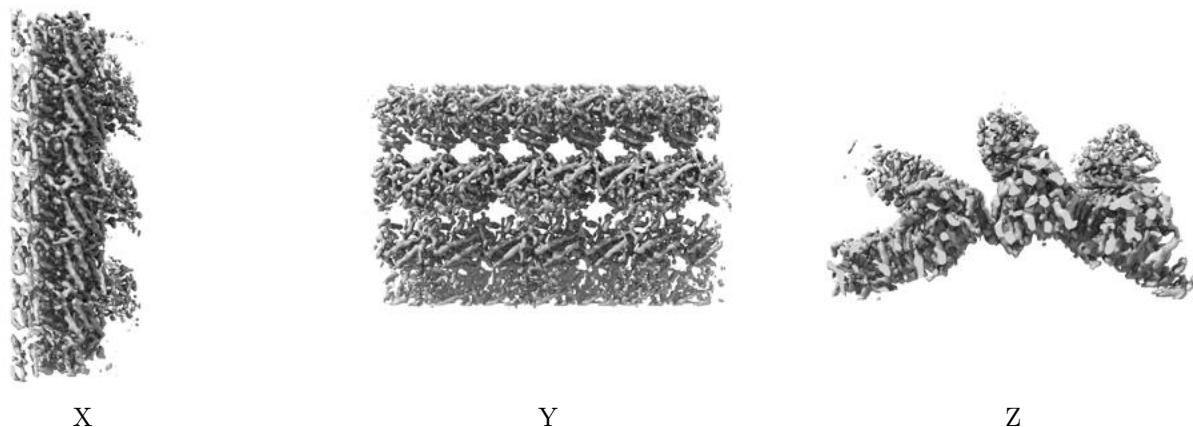


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

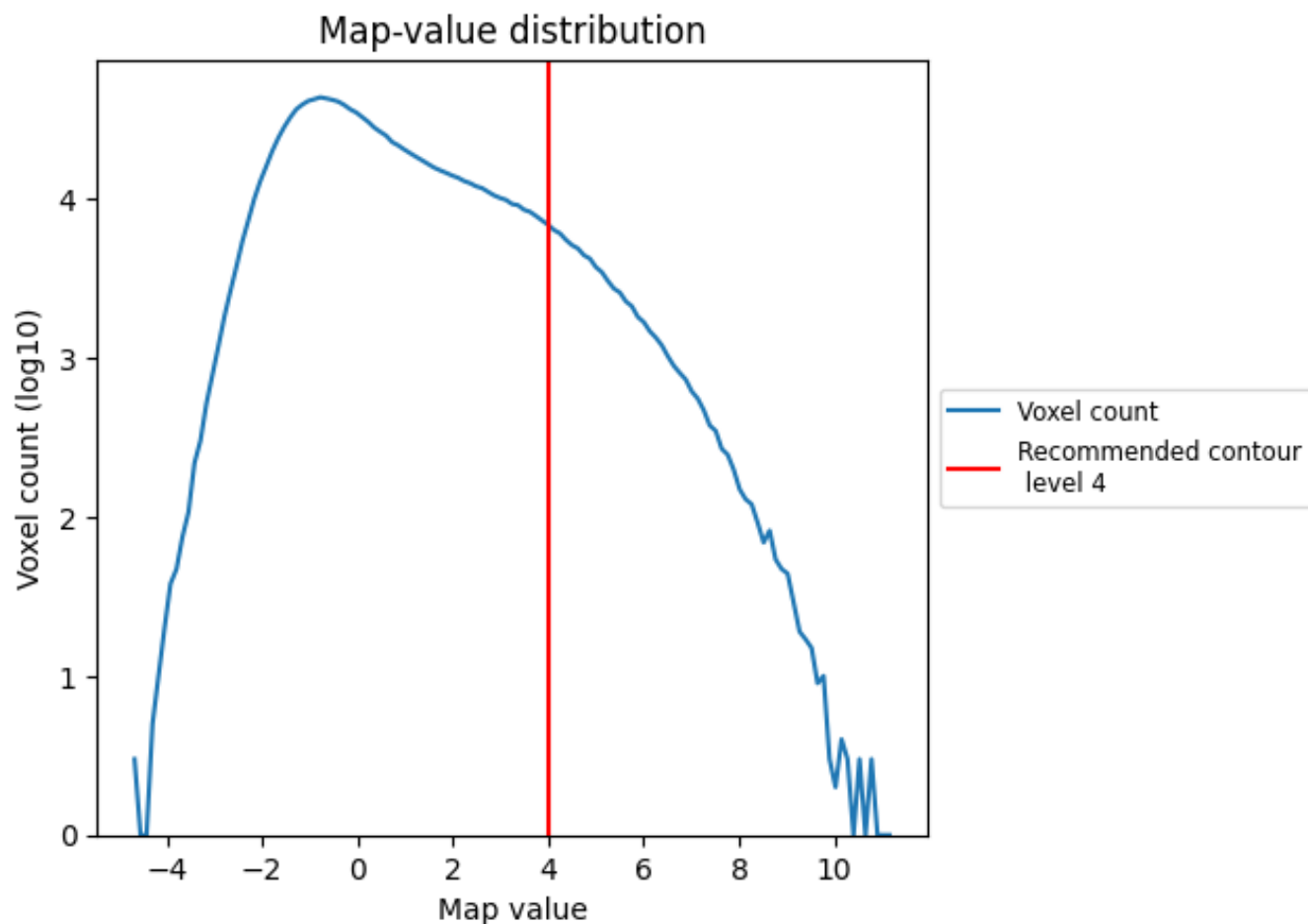
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

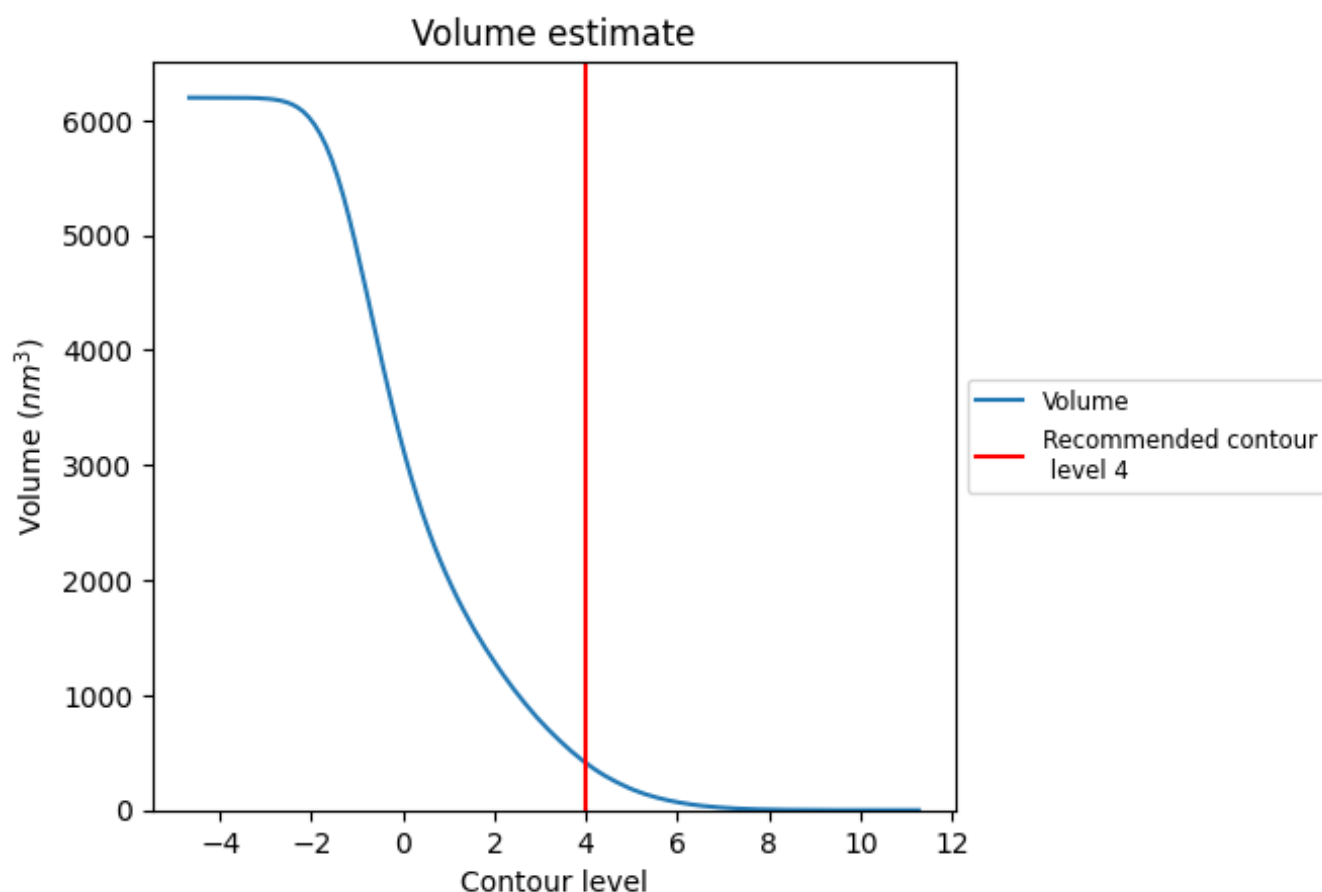
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm³; this corresponds to an approximate mass of 371 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

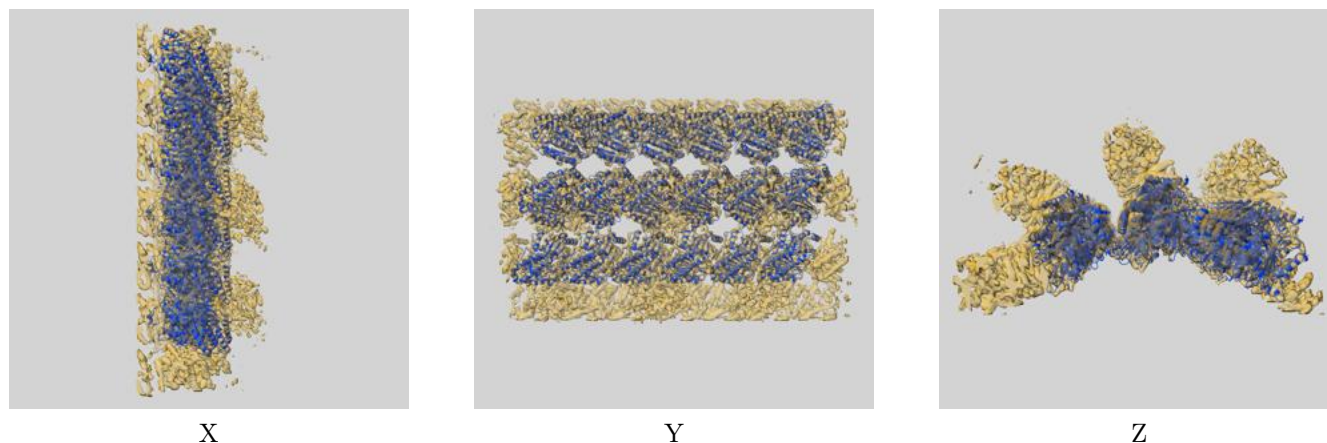
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

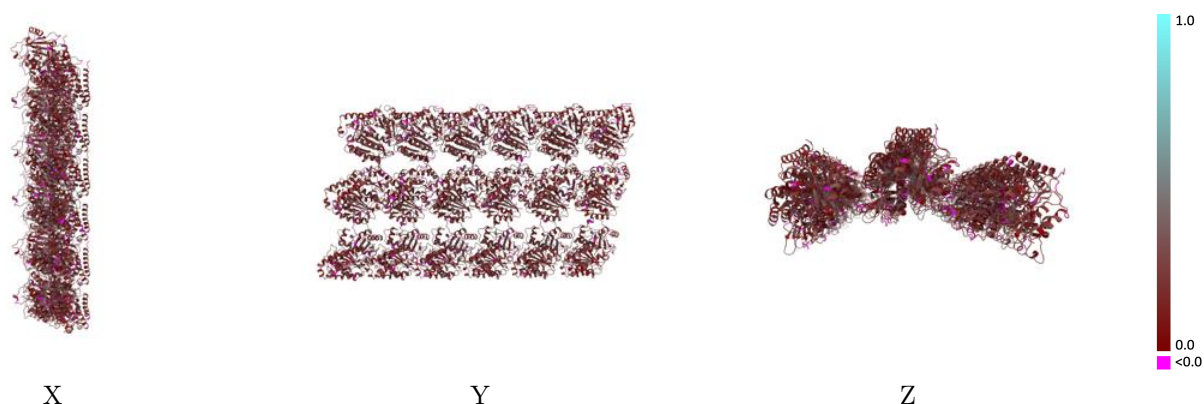
This section contains information regarding the fit between EMDB map EMD-5896 and PDB model 3J6F. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



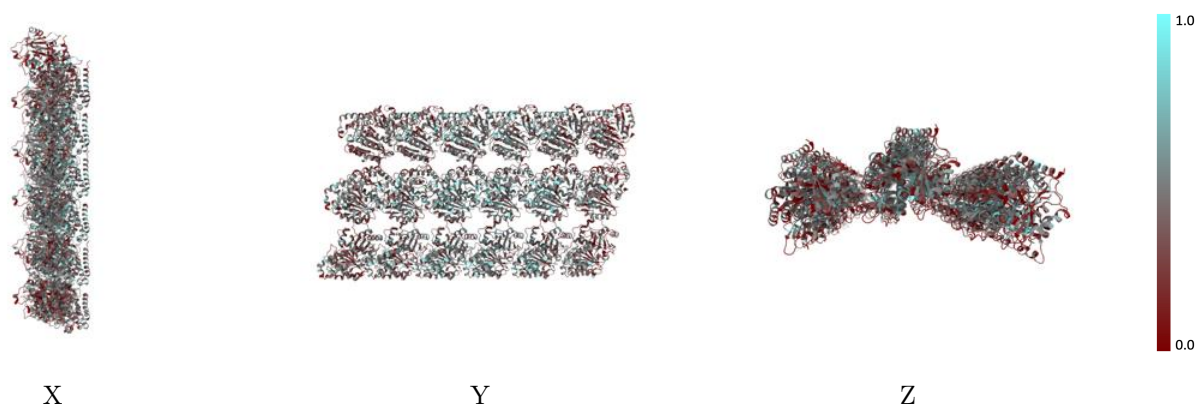
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



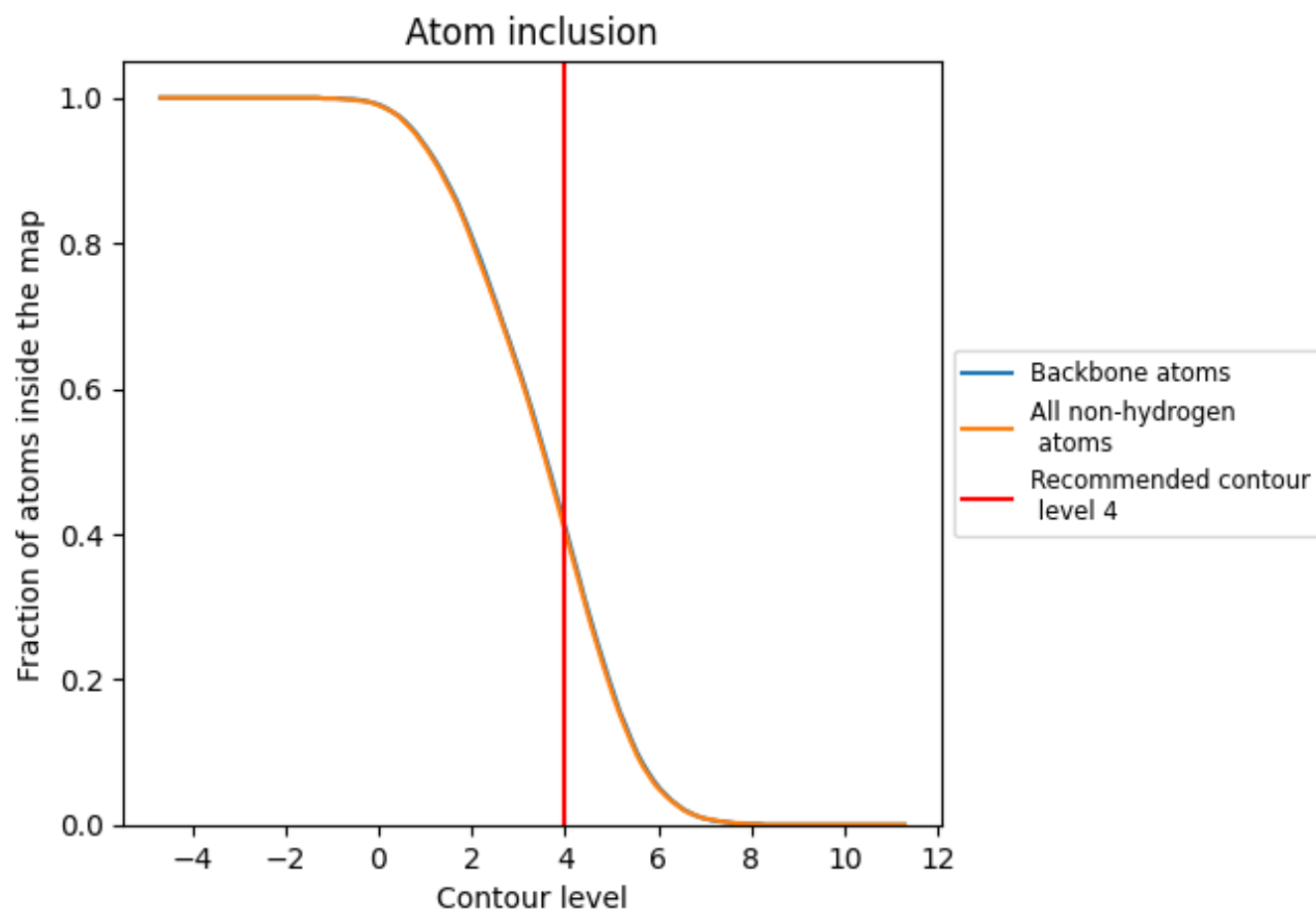
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4040	 0.2220
A	 0.4720	 0.2280
B	 0.4920	 0.2360
C	 0.4320	 0.2210
D	 0.4480	 0.2310
E	 0.4330	 0.2230
F	 0.4530	 0.2350
G	 0.3990	 0.2110
H	 0.3520	 0.2150
I	 0.4380	 0.2160
J	 0.4000	 0.2230
K	 0.4000	 0.2170
L	 0.3500	 0.2170
M	 0.3420	 0.2130
N	 0.4190	 0.2300
O	 0.3770	 0.2110
P	 0.4620	 0.2320
Q	 0.3310	 0.2090
R	 0.4090	 0.2300

